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# Ensemble-Averaged QM/MM Kinetic Isotope Effects for the $S_N2$ Reaction of Cyanide Anion with Chloroethane in DMSO Solution

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**Abstract:** The existence of solvent fluctuations leads to populations of reactant-state (RS) and transition-state (TS) configurations and implies that property calculations must include appropriate averaging over distributions of values for individual configurations. Average kinetic isotope effects ⟨KIE⟩ for $NC^- + EtCl \rightarrow NCEt + Cl^-$ in DMSO solution at 30 °C are best obtained as the ratio $\langle f_{RS}\rangle/\langle f_{TS}\rangle$ of isotopic partition function ratios separately averaged over all RS and TS configurations. In this way the hybrid AM1/OPLS-AA potential yields ⟨KIE⟩ values for all six isotopic substitutions (2° α-$^2H_2$, 2° β-$^2H_3$, α-$^{11}C/^{14}C$, leaving group $^{37}Cl$, and nucleophile $^{13}C$ and $^{15}N$) for this reaction in the correct direction as measured experimentally. These thermally-averaged calculated KIEs may be compared meaningfully with experiment, and only one of them differs in magnitude from the experimental value by more than one standard deviation from the mean. This success contrasts with previous KIE calculations based upon traditional methods without averaging. The isotopic partition function ratios are best evaluated using all (internal) vibrational and (external) librational frequencies obtained from Hessians determined for subsets of atoms, relaxed to local minima or saddle points, within frozen solvent environments of structures sampled along molecular dynamics trajectories for RS and TS. The current methodology may perfectly well be implemented with other QM or QM/MM methods, and thus provides a useful tool for investigating KIEs in relation to studies of chemical reaction mechanisms in solution or catalysed by enzymes.

**Keywords:** computational chemistry • isotope effects • molecular dynamics • solvent effects • transition states

## Introduction

Molecules are constantly in motion. While recognized very clearly by Louis Hammett in his seminal 1940 *Physical Organic Chemistry*,[1] the implications of this fact seem not to have penetrated our understanding of chemistry as widely and deeply as they should have done by now. It is well known that kinetic isotope effects (KIEs), as discussed in this paper, arise predominantly from subtle energetic differences in the quantized internal motions of molecules, due to isotopic substitution, that persist even at 0 K. However, a consequence of external motion of molecules, relative to each other, at non-zero is that many observable properties, including KIEs, are averages over a multitude of thermally accessible configurations of (for example) solvent molecules surrounding one or more solute molecules undergoing a chemical reaction. The purpose of this paper is to demonstrate how explicit sampling of, and averaging over, an ensemble of configurations of a thermally fluctuating molecular system allows calculated KIEs to be reconciled with experiment. In so doing, it suggests a shift away from thinking about chemical change experienced by a single molecule towards a mental picture of a distribution of chemical changes experienced by a representative collection of molecules giving rise to an average value of any property.

KIE measurements are one of the most powerful experimental techniques for probing the nature of the transition state: the magnitude and direction of a KIE contains information about the mechanistic events in a chemical reaction, reflecting differences in bonding between the reactants and the transition state.[2] Quantum-mechanical (QM) techniques are of value to assist interpretation of KIEs,[3] but an important paper by Paneth, Matsson, Westaway (PMW) and their co-workers[4] cast some doubt upon their ability to

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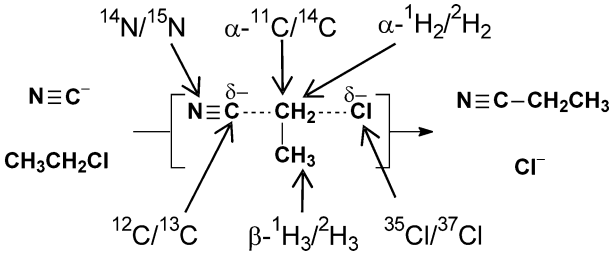
Supporting information for this article (full details of computational procedures, plots of IPFRs and their cumulative means and standard deviations, and Tables of calculated IPFRs for all RS and TS structures) is available on the WWW under http://www.chemeurj.org/ or from the author, from whom also the computer programs for IPFRs are freely available.

reproduce and rationalize experimental KIEs for a prototypical $S_N2$ reaction in solution. These authors' conclusion - that none of the many combinations of QM method and basis set they used was capable of reproducing the range of KIEs measured experimentally for isotopic substitution at six positions (Scheme 1) for reaction of cyanide anion with chloroethane in dimethylsulfoxide (DMSO) – is alarming and sets a challenge for theory. In common with most other KIE calculations,[3] PMW considered only the properties of individual transition structures, but the growing ability of computational chemistry to handle larger systems with increasing intrinsic accuracy means that the reliability of a result is dictated not just by the chosen QM method but also by other factors contingent upon the increase in complexity, dimensionality and flexibility of the system. The dynamics of solvent-solvent and solvent-solute interactions introduce additional issues so that QM methods must be married with techniques of statistical mechanics in order to describe reactivity in condensed phases.




Scheme 1. Isotopic substitutions at six positions within the reactin.

We were among the first to use hybrid QM/MM methods (in which that part of a molecular system involving significant electronic reorganization is described by QM and surrounded by a molecular-mechanical (MM) environment) for KIE calculations with explicit solvation[5] and, along with many other groups,[6] have since used these methods in combination with molecular dynamics (MD) to compute free energy changes from potentials of mean force (PMFs).[7] These studies have established that both reactant states and transition states of large, flexible molecular systems should be modelled by averaging over multiple configurations. In our experience the variation in KIE values calculated with a single QM method (in QM/MM) but with different solvent configurations can be as great as that between different QM methods, suggesting that comparisons of calculated and observed KIEs for reactions in explicit solution are, in general, likely to be either meaningless or fortuitous unless appropriate averaging over solvent configurations is performed. Also, for accurate calculations of secondary alpha-deuterium (2° α-$^2$H) KIEs for reactions in condensed media, we have shown the need to include at least those atoms directly involved in hydrogen bonds to the substrate or, better, a complete first solvation shell within the Hessian used to compute the partition functions for isotopologues.[8]

Our purpose here is to show that theory and experiment may be reconciled for the $S_N2$ reaction of cyanide anion with chloroethane in DMSO (Scheme 1) provided that proper account is taken of thermal fluctuations in solvent configurations by means of appropriate averaging of the computed KIEs. We describe our procedures in detail in order to demonstrate the feasibility and promise of the method rather than as a definitive treatment of the title reaction but nonetheless, despite the known deficiencies of the QM/MM potential (AM1/OPLS-AA) used here, the overall extent of agreement between the resulting ensemble-averaged KIEs and experiment is remarkable. Not only do we succeed in correctly reproducing the direction of all six KIEs, but we gain unprecedented

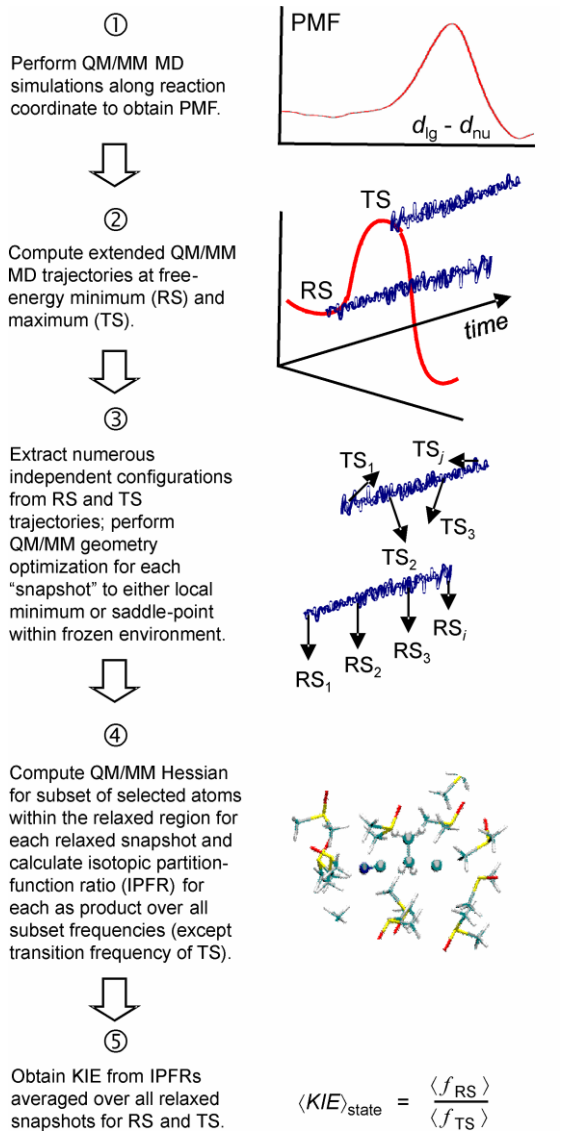



Figure 1. Five steps to ensemble-averaged KIEs.

insight into the sensitivity of KIEs to fluctuations in solvent configuration, revealing surprisingly wide distributions of individual KIE values over which our average values are obtained. Moreover, the conclusion that AM1 overestimates the magnitude of the 2° α-$^2H_2$ KIE relative to experiment is validated by virtue of averaging over many solvent configurations. These findings provide a necessary corrective to the mindset that considers only a single reactant structure (RS) undergoing chemical transformation via a single transition structure (TS) and suggest that, in general, any comparison of condensed-phase experiments with results of a particular QM method may be meaningless unless the calculations include proper averaging.

## Methodology

The key steps (Figure 1) of our procedure for ensemble averaging of KIEs are as follow.

1 Perform QM/MM MD simulations with umbrella sampling along a distinguished coordinate for the reaction at the desired temperature and compute a PMF.

2 At the free-energy minimum (RS) and maximum (TS) of the PMF, compute extended QM/MM MD trajectories; the TS is subject to a constraint to prevent it collapsing to the RS or product.

3 From the RS and TS trajectories, extract numerous independent configurations. For each "snapshot", perform QM/MM geometry optimization to either a local minimum or saddle-point within a frozen environment.

4 Compute the QM/MM Hessian for a subset of selected atoms within the relaxed region and thence the isotopic partition-function ratio (IPFR) for each isotopic substitution of interest.

5 Calculate the average KIE from the IPFRs of all the RS and TS configurations.

Steps 1 – 4 are, in themselves, each quite standard but are discussed in detail below in the Methods section; they are based upon a method for computation of solvent effects on vibrational spectra of stable molecules in solution,[9] but now applied to transition states and KIEs.[10] However, it is appropriate now to describe the non-standard methods used in Stage 5, setting them in the context of other approaches to KIE calculations. Our approach bears similarities with the ensemble-averaged variational transition state theory (EA-VTST) method of Truhlar and co-workers,[11] but differs from it in ways that will be discussed below.

## IPFRS, KIEs and averaging

IPFRs were determined from the coordinates and Hessians of the subsets in either of two ways. The first procedure ignores all coupling between the $N_s$ subset atoms and their environment. The six librational degrees of freedom of the subset with respect to its environment are eliminated by means of a projection method which converts them into translational and rotational modes with zero eigenvalues. This leaves $3N_s - 6$ genuine vibrations which satisfy the Teller-Redlich product rule[12] for isotopologues, being entirely consistent with the masses and moments of inertia obtained from the molecular geometries of the subset atoms alone. This is the "translation/rotation" procedure. The second, simpler, procedure includes all $3N_s$ vibrational modes of the subset: it does not strictly satisfy the Teller-Redlich product rule but neither does it need to do so;[13] this is the "all-frequencies" procedure.

A KIE is an exponential of the difference in activation free energy for an isotopologous pair of reactions. An ensemble average for this quantity could, in principle, be obtained directly by appropriate MD simulations incorporating quantum effects on nuclear motions. In practice it is usual to perform classical MD and then to replace the classical vibrational partition function by the quantum partition function for a set of harmonic oscillators, usually for only a subset of the full system. It is usually considered adequate to treat both translational and rotational motions classically. Within the Born-Oppenheimer approximation, the potential energy barrier is the same for each isotopologue and therefore does not contribute to the difference in activation free energy, which is determined solely by differences in the (natural logarithms of the) partition-functions.

Within transition-state theory, the semiclassical KIE is given by eq. 1, where $Q^{RS}$ and $Q^{TS}$ are molecular partition functions for RS and TS species, respectively. If translations, rotations and vibrations are considered as separable motions, each $Q$ is the product of $q_{trans}$, $q_{rot}$ and $q_{vib}$: the latter term is evaluated over $3N - 6$ modes for RS and but $3N - 7$ modes for TS. Re-arrangement of the partition-function factors on the middle-left-hand side of eq. 1 yields a ratio ("RS over TS") of IPFRs ("heavy over light"), $f_{RS}$ and $f_{TS}$, the values of which should each be always >1. Note that this expression for the KIE does not explicitly include the ratio of isotopic transition frequencies $(\nu_{light}/\nu_{heavy})^{\ddagger}$; its effect is implicitly included within $q_{trans}$ and $q_{rot}$ values for the light and heavy RS and TS species.

$$KIE = \frac{(Q^{TS}/Q^{RS})_{light}}{(Q^{TS}/Q^{RS})_{heavy}} = \frac{(Q_{heavy}/Q_{light})^{RS}}{(Q_{heavy}/Q_{light})^{TS}} = \frac{f_{RS}}{f_{TS}} \quad (1)$$

It is common for the Teller-Redlich product rule to be employed in order to replace the $q_{trans}$ and $q_{rot}$ factors, involving masses and moments-of-inertia, by a factor involving only products of vibrational frequencies for the light and heavy species; these products are taken over all $3N - 6$ modes for both RS and TS. However, in the Bigeleisen equation (eq. 2) for the KIE,[14] the vibrational products are included along with the $q_{vib}$ factors in a representation (where $u = hc\nu/k_BT$) which runs over $3N - 7$ modes for TS; this means that the ratio of the transition frequencies appears explicitly as an extra factor. The Bigeleisen equation may also be re-arranged as a ratio of IPFRs evaluated using vibrational frequencies only, but note that here the TS value involves products over only $3N - 7$ frequencies, so that $f_{TS} = (\nu_{heavy}/\nu_{light})^{\ddagger} \times f_{\ddagger}$.

$$KIE = \left[\frac{\nu_{light}}{\nu_{heavy}}\right]^{\ddagger} \prod_{i}^{3N-6}\left[\frac{\nu_i^{RS}\sinh(u_i^{RS}/2)_{light}}{\nu_i^{RS}\sinh(u_i^{RS}/2)_{heavy}}\right] \prod_{i}^{3N-7}\left[\frac{\nu_i^{TS}\sinh(u_i^{TS}/2)_{light}}{\nu_i^{TS}\sinh(u_i^{TS}/2)_{heavy}}\right] \quad (2)$$

$$KIE = \left[\frac{\nu_{light}}{\nu_{heavy}}\right]^{\ddagger} \frac{f_{RS}}{f_{\ddagger}} \quad (3)$$

We have recently pointed out[13] that, since the Teller-Redlich product rule applies only when translational, rotational and vibrational motions are separable – which is not true for subsets of atoms within the environment of a larger system, the Bigeleisen equation in its conventional form is inappropriate for use in conjunction with subset Hessians. Instead we have shown[13] that the product of all $3N_s$ harmonic vibrational frequency ratios for a pair of isotopologues is equal simply to the product of isotopic mass ratios, for the isotopically substituted atoms only, raised to the power of 3/2; moreover, these terms are identical for both RS and TS and therefore disappear from the KIE (eq. 4). For reasons discussed below, it is convenient to use IPFRs in order to evaluate ensemble-averaged KIEs for systems described by subset Hessians; these are given by eqs. 5 and 6, in which the isotopic mass-ratio factors are retained solely for comparability with IPFR values obtained by means of the Bigeleisen equation.

$$KIE = \prod_{i}^{3N_s} \frac{\sinh(u_i^{RS}/2)_{light}}{\sinh(u_i^{RS}/2)_{heavy}} \prod_{i}^{3N_s-1} \frac{\sinh(u_i^{TS}/2)_{light}}{\sinh(u_i^{TS}/2)_{heavy}} \quad (4)$$

$$(f_{RS})_{subset} = \left[\prod_{j}^{N_{iso}} \frac{(m_j)_{light}}{(m_j)_{heavy}}\right]^{\frac{3}{2}} \prod_{i}^{3N_s} \frac{\sinh(u_i^{RS}/2)_{light}}{\sinh(u_i^{RS}/2)_{heavy}} \quad (5)$$

$$(f_{TS})_{subset} = \left[\prod_{j}^{N_{iso}} \frac{(m_j)_{light}}{(m_j)_{heavy}}\right]^{\frac{3}{2}} \prod_{i}^{3N_s-1} \frac{\sinh(u_i^{TS}/2)_{light}}{\sinh(u_i^{TS}/2)_{heavy}} \quad (6)$$

Two approaches are considered for obtaining average values of the KIEs from the sets of RS and TS Hessians. The first takes all possible combinations of the $\Omega_{RS}$ reactant structures (i) and Hessians with the $\Omega_{TS}$ transition structures and Hessians (j): an individual isotope effect $KIE_{ij}$ (eq. 7) is computed for each pair, and the average $\langle KIE\rangle_{indiv}$ is found as the arithmetic mean (eq. 8) of all $\Omega_{RS} \times \Omega_{TS}$ individual values.

$$KIE_{ij} = (f_{RS})_i / (f_{TS})_j \quad (7)$$

$$\langle KIE \rangle_{\text{indiv}} = \frac{1}{\Omega_{RS} \times \Omega_{TS}} \sum_{i}^{\Omega_{RS}} \sum_{j}^{\Omega_{TS}} KIE_{ij} \quad (8)$$

The second approach considers all $\Omega_{RS}$ reactant structures as a reactant-state ensemble and all $\Omega_{TS}$ transition structures as a transition-state ensemble: the average $\langle KIE \rangle_{\text{state}}$ (eq. 11) is obtained as the quotient of the average IPFR for the transition state (eq. 9) as dividend with the average IPFR for the reactant state (eq. 10) as divisor.

$$\langle f_{RS} \rangle = \frac{1}{\Omega_{RS}} \sum_{i}^{\Omega_{RS}} (f_{RS})_i \quad (9)$$

$$\langle f_{TS} \rangle = \frac{1}{\Omega_{TS}} \sum_{j}^{\Omega_{TS}} (f_{TS})_j \quad (10)$$

$$\langle KIE \rangle_{\text{state}} = \langle f_{RS} \rangle / \langle f_{TS} \rangle \quad (11)$$

Both methods are based on the assumption that the reactant state and the transition state are entirely independent; this means that there is an equal probability of each and every individual reactant structure going to each and every individual transition structure. This assumption is entirely consistent with conventional transition-state theory but could be inappropriate if relaxation of the solvent environment were slow compared with the chemical reaction step. If KIEs were computed for pairs of RS and TS directly connected by an individual intrinsic reaction coordinate path (*cf.* ref. 11), it would not be obvious what the appropriate method for averaging should be, since there would not be an equal probability for each path. The RS and TS structures in this work are selected from MD trajectories which should already each reflect a Boltzmann distribution. In the present study the number of solvent molecules included in the Hessian for each individual RS and TS varies from 0 to 10, and therefore the molecular partition functions $Q^{RS}$ and $Q^{TS}$ vary very considerably in magnitude and would not be amenable to meaningful averaging over the $\Omega_{RS}$ or $\Omega_{TS}$ values. However, it is meaningful to consider the IPFRs as the basis for averaging, since variation in these quantities does not show any obvious dependence on the number of solvent molecules included in the Hessian.

Within the limits of the harmonic approximation adopted for the "all-frequencies" method for evaluating IPFRs, and thence KIEs, it is logical to include a quantum correction to the partition function not only for each separable vibrational mode with a real frequency (*i.e.* zero-point energy) but also for motion in the transition vector with its imaginary frequency (*i.e.* tunnelling). The tunnelling correction to the KIE may be obtained simply (albeit approximately) by means of Bell's expression[15] for an inverted parabola, eq. 12.

$$KIE_{\text{corr}} = \left[\frac{\nu_{\text{light}}}{\nu_{\text{heavy}}}\right]^{\ddagger} \frac{\sin(u_i^{TS}/2)_{\text{heavy}}}{\sin(u_i^{TS}/2)_{\text{light}}} \frac{(f_{RS})_{\text{subset}}}{(f_{TS})_{\text{subset}}} \quad (12)$$

In the event that the relaxation of the subset atoms to a local minimum or saddle point within their frozen environment yielded any residual small imaginary frequencies (not including the transition frequency for a transition structure), we treated these in either of two ways. Firstly, any small imaginary frequency was replaced by a real frequency of the same magnitude. Alternatively, any small imaginary frequency was simply omitted[16] from the evaluation of the vibrational partition functions (eqs. 5 and 6) which therefore involved products over correspondingly fewer than $3N_s$ or $3N_s - 1$ frequencies.

## Results and Discussion

**Stages 1 - 3.** The free energy of activation (~142 kJ mol$^{-1}$ at 300 K) obtained from the AM1/OPLS-AA PMF is higher than either the experimental value[3] (94.6 kJ mol$^{-1}$) or the *ab initio* PCM/CCSD(T)/6-311+G(2df,2p)//B3LYP/6-31G(d) estimate of $\Delta G^{\ddagger}$ = 101 kJ mol$^{-1}$ for this reaction in DMSO.[17] Although AM1 gives erroneous energies, possible errors in computed KIEs are likely to be much smaller owing (in part) to their nature as exponentials of free-energy differences due to isotopic shifts.

The mean values of the making and breaking bond distances in the 100 TS structures are $C_\alpha$–$C_{nu}$ = 2.08 ± 0.05 Å and $C_\alpha$–Cl = 2.12 ± 0.04 Å and the mean of the $C_{nu}$–$C_\alpha$–Cl angle is 166° ± 2°, indicating that these key structural parameters of the transition state are well defined. The same is not true for the "reactant complex" structures determined, starting from the free-energy minimum in the PMF profile, by means of energy minimization within a frozen environment but without constraints upon the cyanide and chloroethane moieties (or on DMSO molecules in the first solvation shell): the average value of the distance $C_\alpha \cdots C_{nu}$ to the nucleophile in these 100 structures is very long (7.733 ± 1.713 Å) with a very large standard deviation. The actual reagent used in the experimental study was tetra-*n*-butylammonium cyanide,[3] and a conductometric study[18] has shown that there is no ion pairing between *n*-$Bu_4N^+$ and $NC^-$ in DMSO at 25 °C; this result implies that no significant amount of association between $NC^-$ and EtCl should be expected in DMSO solution at 300 K. Inspection of each of the 100 "reactant complex" structures also reveals no evidence for any precursor ion-molecule complex ($NC^- \cdots$EtCl): the cyanide and chloroethane moieties are independently solvated and randomly oriented relative to each other. Consequently we decided to take these 100 structures together with another 100 structures for solvated $NC^-$ by itself and 100 structures for solvated EtCl by itself as part of a single ensemble of reactant-state structures RS. Furthermore, a fraction of the locally-minimized AM1/OPLS-AA structures for solvated cyanide anion showed unrealistic bonding motifs (*e.g.* formation of a covalent adduct with DMSO); 122 RS structures remained after removal of these non-physical configurations.

**Kinetic isotope effects without explicit solvation.** It is helpful first to establish how the AM1 method performs for KIE calculations in a vacuum and in continuum solvent. Neither method predicts the direction (normal or inverse) of all six KIEs (Table 1, rows 1 and 2), although the PCM description of DMSO does better; neither method is correct for $k_H/k_{\beta\text{-}^2H_3}$, and PCM is incorrect for $k^{35}{}_{Cl}/k^{37}{}_{Cl}$. Whilst the inverse sense of $k_H/k_{\alpha\text{-}^2H_2}$ is correctly predicted by AM1, its magnitude (deviation from unity) is too large. Interestingly, not only does the M06-2X/6-31+G(d,p)/PCM method overcorrect this KIE, predicting a small normal value (Table 1, row 3), but also it incorrectly predicts inverse values for $k_H/k_{\beta\text{-}^2H_3}$, $k^{12}{}_C/k^{13}{}_{C_{nu}}$ and $k^{14}{}_N/k^{15}{}_{N_{nu}}$.

**Average kinetic isotope effects with explicit solvation.** The most striking point to notice from the AM1/OPLS-AA ensemble-averaged KIEs (Table 1) is that, regardless of which averaging method is used, there is qualitative agreement (normal or inverse) with the experimental values[4] for all six different isotopic substitutions. PMW[4] considered 39 different combinations of QM method and basis set available within Gaussian98, and other

Table 1. Mean values and standard deviations (1σ) of averaged kinetic isotope effects for $S_N2$ reaction $NC^-$ + EtCl in DMSO. [a]

| description | reactants | $T$ / K | $k_H/k_{\alpha\text{-}D_2}$ | $k_H/k_{\beta\text{-}D_3}$ | $k^{11}C_\alpha/k^{14}C_\alpha$ | $k^{35}Cl/k^{37}Cl$ | $k^{12}C_{nu}/k^{13}C_{nu}$ | $k^{14}N/k^{15}N$ |
|---|---|---|---|---|---|---|---|---|
| *Vacuum or continuum solvation:* | | | | | | | | |
| $KIE_{vacuum}$ | separate | | 0.920 | 0.989 | 1.20 | 1.0075 | 0.9870 | 0.9993 |
| $KIE_{PCM}$ | separate | | 0.916 | 0.982 | 1.19 | 0.9927 | 1.0018 | 1.0014 |
| $KIE_{M06\text{-}2X}$ [b] | separate | | 1.043 | 0.964 | 1.19 | 1.0068 | 0.9917 | 0.9989 |
| *Translation/rotation procedure: librational modes replaced by translations and rotations:* | | | | | | | | |
| $\langle KIE\rangle_{indiv}$ | separate | 300 | 0.934 ± 0.023 | 1.012 ± 0.025 | 1.207 ± 0.002 | 1.0048 ± 0.0065 | 1.0022 ± 0.0083 | 1.0028 ± 0.0044 |
| $\langle KIE\rangle_{state}$ | separate | 300 | 0.934 ± 0.023 | 1.012 ± 0.025 | 1.207 ± 0.002 | 1.0048 ± 0.0065 | 1.0022 ± 0.0083 | 1.0028 ± 0.0045 |
| *All-frequencies procedure: librational modes treated as harmonic vibrations; extra imaginaries replaced by real frequencies:* | | | | | | | | |
| $\langle KIE\rangle_{indiv}$ | RS | 300 | 0.921093 ± 0.020584 | 1.004112 ± 0.023234 | 1.191894 ± 0.005771 | 1.007237 ± 0.000321 | 1.000246 ± 0.008029 | 1.001740 ± 0.002079 |
| $\langle KIE\rangle_{state}$ | RS | 300 | 0.920819 ± 0.02310 | 1.003877 ± 0.023605 | 1.191893 ± 0.005312 | 1.007244 ± 0.000478 | 1.000245 ± 0.008126 | 1.001742 ± 0.002068 |
| $\langle KIE\rangle_{state}$ | RS | 303.15 | 0.921 ± 0.020 | 1.006 ± 0.023 | 1.190 ± 0.005 | 1.0071 ± 0.0005 | 1.0006 ± 0.0076 | 1.0014 ± 0.0016 |
| $\langle KIE_{corr}\rangle_{state}$ | RS | 303.15 | 0.923 ± 0.020 | 1.014 ± 0.023 | 1.268 ± 0.018 | 1.0081 ± 0.0005 | 1.0032 ± 0.0079 | 1.0032 ± 0.0017 |
| *All-frequencies procedure: librational modes treated as harmonic vibrations; extra imaginaries omitted:* | | | | | | | | |
| $\langle KIE\rangle_{state}$ | RS | 303.15 | 0.921 ± 0.021 | 1.008 ± 0.031 | 1.190 ± 0.009 | 1.0077 ± 0.0047 | 1.0007 ± 0.0076 | 1.0014 ± 0.0023 |
| *Experiment:* [c] | | | | | | | | |
| | separate | 303.15 | 0.990 ± 0.004 | 1.014 ± 0.003 | 1.21 ± 0.02 | 1.0070 ± 0.0003 | 1.0009 ± 0.0007 | 1.0002 ± 0.0006 |
| $N$ [d] | | | 4 | 3 | 12 | 8 | 18 | 14 |

[a] The number of decimal places shown for both means and standard deviations in several of the rows of this Table deliberately exceeds the number of significant figures as judged by the magnitude of those standard deviations (see text for discussion). [b] M06-2X/6-31+G(d,p)/PCM. [c] Ref. 3. [d] Number of independent experiments used to determine mean value and standard deviation of KIE.

programs for electronic structure calculations, but none of those methods predicted the direction of the isotope effect in agreement with experiment for all six substitutions. (Quantitatively, it is clear that the α-$^2H_2$ KIE is seriously in error: see below.) It is perhaps significant that no explicit DMSO molecules were included in that study, and certainly there was no ensemble averaging of solvent configurations. In a subsequent paper PMW and their co-workers[19] studied the same reaction in THF solvent in order to test whether the discrepancy between the TS structures predicted by their calculations[4] and by their interpretation of the experimental KIEs, and they concluded that the lack of solvation in the calculations was not responsible. The present results call this conclusion into question, and suggest that it would be of interest also to perform these simulations with ensemble averaging in THF for comparison.

The standard deviations for the calculated ensemble-averaged KIEs do not have the same significance as those reported for the experimental values. The calculated standard deviations reflect the breadth of the distribution of precisely computed IPFRs for each individual relaxed snapshot within a limited sample of RS and TS configurations spanning a range of structures determined by the model potential, whereas the experimental errors arise from uncertainties in rate-constant determinations for (effectively) complete sampling of all thermally accessible RS and TS configurations which may also span a distribution of structures. Notwithstanding this important proviso, the calculated and experimental KIEs (Table 1) agree within the degree of uncertainty of a single standard deviation (1σ) for all methods for each of the isotopic substitutions except $k_{\alpha\text{-}^1H_2}/k_{\alpha\text{-}^2H_2}$. Although in the latter case the experimental value is an average of only four determinations, it is probably safe to conclude that the calculated results for α-deuterium substitution are indeed too large in the inverse sense. With this exception, the overall extent of agreement between ensemble-averaged AM1/OPLS-AA KIEs and experiment is remarkable, despite the acknowledged deficiencies of the method in regard to computed energies. Only one [MP2/6-31+G(d,p)] of the 39 methods considered by PMW yielded calculated KIEs that agreed within 1σ for more than three of the six experimental values.[4] According to the ranking scheme used by PMW (based on the sum of absolute errors between calculation and experiment), the best set of results in Table 1 (row 8) is only middle-ranking as assessed by all six KIEs but is table-topping if the 2° α-$^2H_2$ KIE is excluded.

The mean values for $k^{12}C_{nu}/k^{13}C_{nu}$, $k^{14}N/k^{15}N$ and $k^{35}Cl/k^{37}Cl$ calculated by the "translation/rotation" method (Table 1, rows 4 and 5) each differ from experiment by more than those calculated by the "all-frequencies" method. The use of small subset Hessians involving restricted selections of atoms gives rise to errors in IPFRs and KIEs: elsewhere we have recently argued that these errors are considerably smaller for the "all-frequencies" method than for the "translation/rotation" method.[13] The additional computational expense involved in projecting out the six librational modes of the subset and replacing them by translations and rotations is not justified by any improvements in accuracy or precision. Consequently we now only recommend use of the "all-frequencies" method.

The two averaging methods (eqs. 8 and 11) are mathematically different and indeed yield very slightly different means and standard deviations if enough decimal places are considered (Table 1, rows 6 and 7); however, they are indistinguishable if the number of significant figures is restricted to what is justified by the magnitudes of the standard deviations. (The number of decimal places shown for both means and standard deviations in several of the rows of this Table exceeds the number of significant figures. This is done

deliberately in order to allow for comparison between the methods. Once the best method has been established, the results should not be quoted with more than the correct number of significant figures.)

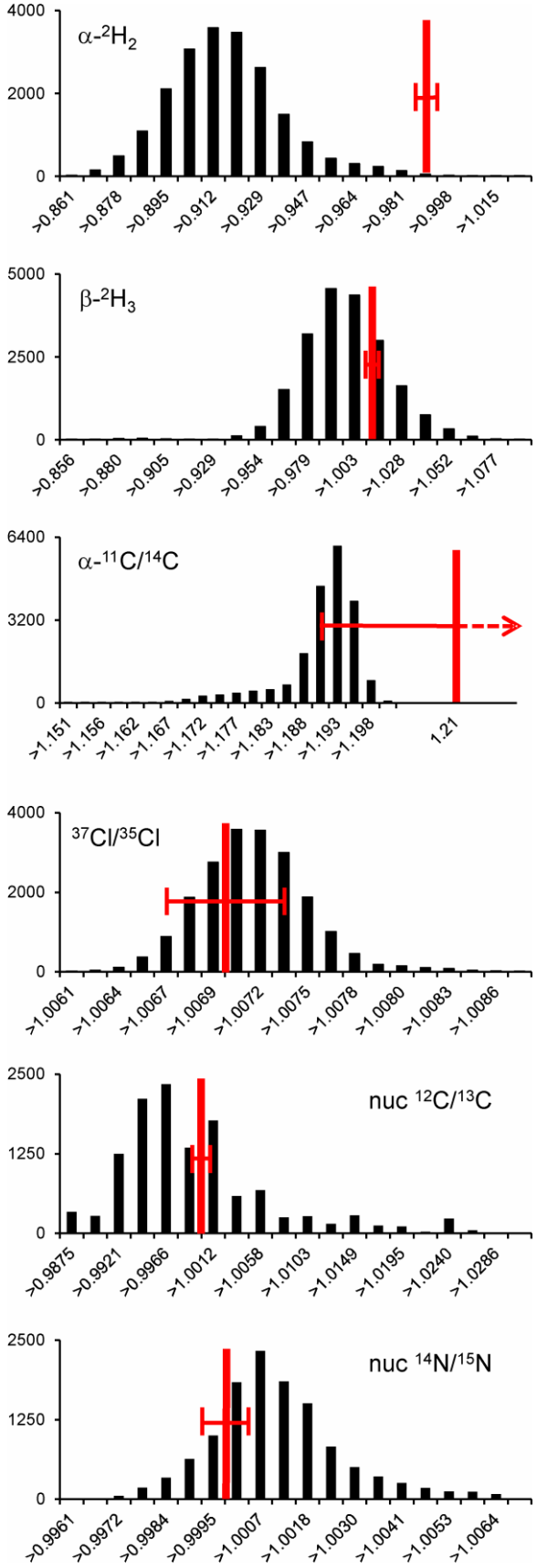



Figure 2. Distributions of individual $KIE_{ij}$ values calculated by the all-frequencies method for $NC^-$ + EtCl in DMSO at 300 K; experimental means and 1σ shown in grey.

The effect of the small difference in temperature between 300 and 303.15 K is entirely as expected: the KIEs are slightly smaller in magnitude (less different from unity) at the higher temperature. The sensitivity of the IPFRs themselves (see Supporting Information) to temperature is more dramatic.

A small proportion of the locally relaxed snapshot structures produced one or more unwanted small imaginary frequencies, representing less than 0.2% of all the computed vibrational frequencies. However, the IPFRs values resulting from replacement of these extra imaginaries by real frequencies of the same magnitude are not abnormal and cannot be recognized as outliers in the distributions (see below). These structures are all included in the results presented in Table 1. Although there is little difference between the KIEs obtained either by replacing these extra imaginaries or by omitting them (*e.g.* compare rows 8 and 10 of Table 1), we recommend the former procedure for the following reason: owing to the non-separability of the internal and external modes, some of these small imaginary frequencies are isotopically sensitive to a (perhaps) surprising extent, such that their omission can cause the IPFR for that particular configuration to become <1, which is unphysical and incorrect. Furthermore, omission leads to larger standard deviations in the IPFR values (see Supporting Information) and KIEs, whereas replacement by real frequencies appears to capture the isotopic sensitivity correctly and ensures that the vibrational product of all $3N_s$ isotopic frequency ratios is numerically equal to the isotopic mass-ratio factor (appearing in eqs. 5 and 6) as it is required to be.

Finally, inclusion of the simple quantum correction for motion in the transition vector (eq. 12) does not lead to general improvement in the agreement between the calculated average KIEs ($\langle KIE_{corr}\rangle_{state}$, Table 1, row 9) and the experimental values.

Bearing in mind all of the above remarks, the "best" results are those from the state-averaged method (eq. 11) with the "all-frequencies" procedure and extra imaginaries replaced by real frequencies: $k_H/k_{\alpha\text{-}^2H_2} = 0.92 \pm 0.02$, $k_H/k_{\beta\text{-}^2H_3} = 1.01 \pm 0.02$, $k^{11}C_\alpha/k^{14}C_\alpha = 1.190 \pm 0.005$, $k^{35}Cl/k^{37}Cl = 1.0071 \pm 0.0005$, $k^{12}C_{nu}/k^{13}C_{nu} = 1.001 \pm 0.008$, and $k^{14}N/k^{15}N = 1.0014 \pm 0.0016$.

**Analysis of isotope effect distributions.** It is of interest to inspect the distributions of individual $KIE_{ij}$ values that contribute to the $\langle KIE\rangle_{indiv}$ average for each of the isotopic substitutions: Figure 2 shows histograms of the number of semi-classical $KIE_{ij}$ values (at 300 K) in small ranges of the $k_{light}/k_{heavy}$ ratios calculated with respect to the combined reactants RS. The distributions for $k_H/k_{\alpha\text{-}^2H_2}$, $k_H/k_{\beta\text{-}^2H_3}$, $k^{11}C_\alpha/k^{14}C_\alpha$ and $k^{35}Cl/k^{37}Cl$ appear more or less symmetrical and bell-shaped, as would be expected for normal distributions. However, the distributions for $k^{12}C_{nu}/k^{13}C_{nu}$ and $k^{14}N/k^{15}N$ are certainly not normal and seem to be comprised of (at least) two overlapping populations; consequently, the means and standard deviations reported in Table 1 must be treated with caution, since they do not refer to normal distributions.

The grey lines in Figure 2 indicate the means and reported standard deviations for the experimental KIEs. Clearly the calculated and experimental distributions for $k_H/k_{\alpha\text{-}^2H_2}$ do not overlap, whereas the experimental values for $k_H/k_{\beta\text{-}^2H_3}$ and $k^{35}Cl/k^{37}Cl$ lie entirely within the range of the calculated distributions. Although the experimental mean for $k^{11}C_\alpha/k^{14}C_\alpha$ differs from the calculated mean, most of the calculated distribution lies within the wide range of the experimental 1σ. This KIE has the largest ratio of transition frequencies (average value of $[\nu^{11}C/\nu^{14}C]^{\ddagger} = 1.09$) and thence the largest quantum correction (1.067 ± 0.015); although the latter may be overestimated by eq. 12, it is possible that a more complete

treatment of tunneling might bring the calculated and experimental KIEs into better agreement.

**Analysis of ln(IPFR) distributions.** It is also very revealing to inspect the distribution of values of IPFRs $f_{RS}$ and $f_{TS}$ that contribute to the averages. Simple plots of each IPFR against its number in the sequence of snapshots do not show any significant upward or download trends away from the mean values, and therefore indicate that the equilibration is adequate. Figure 3 shows histograms of the natural logarithms $\ln(f_{RS})_{subset}$ and $\ln(f_{TS})_{subset}$ for these quantities computed for isotopologous pairs of 122 or 200 locally-relaxed RS (left) and 100 locally-relaxed TS (right) configurations in DMSO at 300 K. It is more meaningful to consider logarithms rather than the IPFRs themselves, since the former reflect differences in free energy. The envelope of each histogram is less smooth than is found, in general, for the distributions of the individual $KIE_{ij}$ values because the population size is 100 times smaller. Even so, the distributions of $\ln(f_{RS})_{subset}$ and $\ln(f_{TS})_{subset}$ for $k_H/k_{\alpha\text{-}^2H^2}$, $k_H/k_{\beta\text{-}^2H_3}$ and $k^{35}Cl/k^{37}Cl$ also appear more or less normal. The distribution for $k^{11}C_\alpha/k^{14}C_\alpha$ shows one low-valued outlier for RS and a tail on the high-valued side for TS which together account for the low-valued tail in the $KIE_{ij}$ distribution for this isotope effect. Simple consideration of the difference between the modes (as opposed, properly, to the means) of the $\ln(f_{RS})_{subset}$ and $\ln(f_{TS})_{subset}$ histograms reveals whether the average KIE is normal or inverse for these isotopic substitutions.

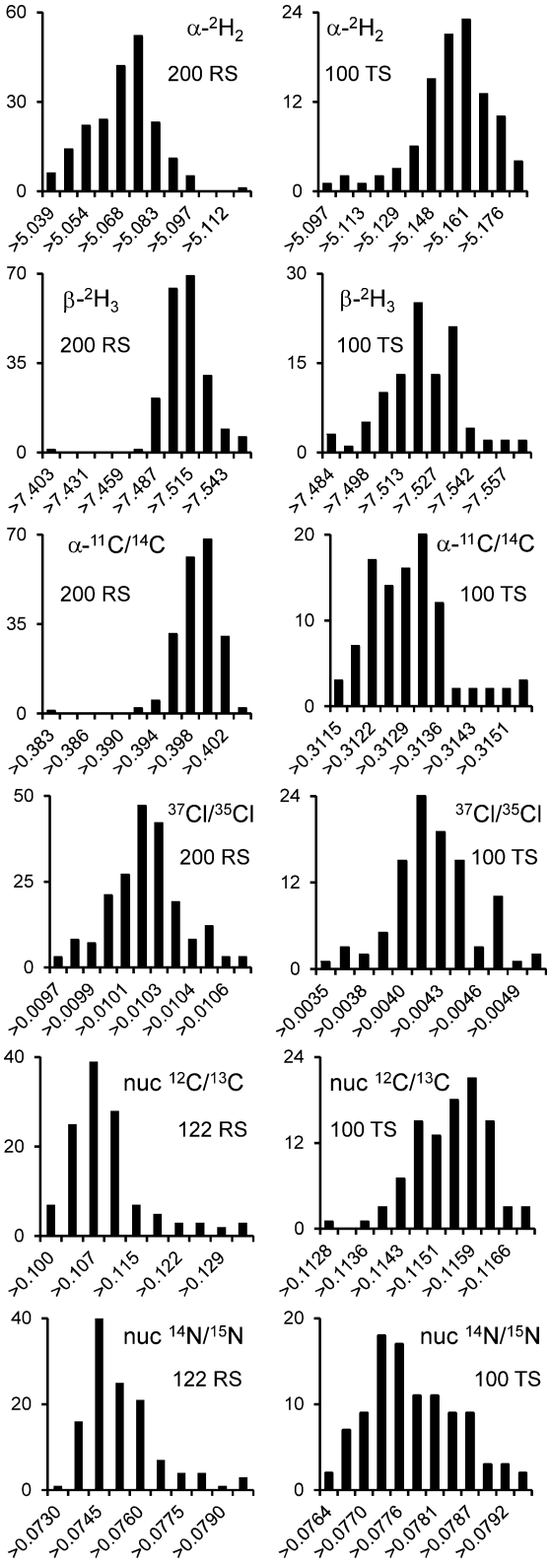



Figure 3. Distributions of natural logarithms of isotopic partition-function ratios for isotopologous pairs of locally-relaxed RS (left) and TS (right) configurations in DMSO at 300 K.

**Relationship to other methods for KIE calculations.** A virtue of the approach described in this paper is that it opens the mind as to how a fluctuating solvent environment gives rise to a whole distribution of KIE values, and therefore provides a necessary corrective to the mindset that considers only a single reactant structure undergoing chemical transformation via a single transition structure. It also makes a more general point that any comparison of condensed-phase experiments with results of a particular QM method is meaningless unless the calculations include proper averaging.

Singleton and co-workers[3] have reported KIEs calculated by means of the Bigeleisen equation (eq. 2) with simple tunnelling (eq. 12) for a range of PCM-optimized TS conformations and have discussed errors associated with non-zero frequencies for external degrees of freedom, but not in the context of subset Hessians; they have also reported the use of Boltzmann-weighted IPFRs in KIE calculations involving a small number of low-energy RS conformations.[20] The second step of the first stage of the EA-VTST method of Truhlar and co-workers[11] involves averaging of vibrational frequencies over a set of configurations in order to convert a classical PMF to one with $3N - 7$ quantized nuclear motions in order to include zero-point and thermal energies: the six lowest-frequency modes are omitted on the grounds that the harmonic approximation is not applicable to these librational motions.[21] We have argued elsewhere that treating them as harmonic vibrations incurs much less error in IPFRs and KIEs than regarding them as classical rotations and translations.[13] The second stage of the EA-VTST method is similar to our procedure in that it involves relaxation of a mobile subset of atoms to a local saddle point within a frozen environment (primary and secondary zones in Truhlar's terminology)[11] to generate a TS ensemble for which the vibrational free energy is computed for $3N_s - 1$ modes. It differs from our procedure, however, in that a minimum-energy path is obtained linking each member of the TS ensemble to a particular RS structure, and the averaging is performed over the activation free energies.[11] The path-integral/free-energy perturbation and umbrella sampling (PI-FEP/UM) method of Major and Gao[22] includes quantization in all degrees of freedom for a small number (typically four) of atoms including the site of isotopic substitution and its immediate neighbours, yielding both zero-point energy and tunnelling effects at the same time; a double averaging is performed to obtain both the

classical PMF and the quantum-mechanical correction along the classical path, and their bisection sampling method allows the Boltzmann-weighted free-energy difference between light and heavy isotopologues to be obtained from the same simulation by FEP in mass from the light to the heavy isotope. By avoiding separate simulations for each isotopologue, this method is capable of yielding both primary and secondary KIEs with acceptably small errors; presumably, however, in view of the small number of quantized atoms, determination of KIEs for multiple isotopic substitutions requires multiple (expensive) PI-FEP/UM simulations. In a sense, our use of the same Hessian for both isotopologues may also be considered as a one-step FEP in mass, albeit within the limitations of the harmonic approximation, and which requires only diagonalization of the subset Hessian for each additional isotopologue.

## Methods

Full details of the computational procedures employed in each step of our procedure are provided in the Supporting Information, but key points are highlighted here.

Hessians for subsets of selected atoms relaxed to a local stationary point within a frozen environment were computed using full QM/MM gradient vectors for the entire system. KIEs were obtained as ratios of IPFRs for RS and TS, which were calculated in two different ways. On the one hand, our CAMVIB and CAMVIB programs were employed, first to remove translational and rotational contributions from computed subset Hessians by a projection method,[23] and second to evaluate partition functions for translation, rotation and vibration of the subset atoms, and thence KIEs, within the harmonic-oscillator, rigid-rotor, ideal-gas approximations and the standard transition-state theory of isotope effects.[2] On the other hand, IPFRs for the subset atoms were determined treating both the internal and external degrees of freedom as harmonic vibrational modes, by means of a new program UJISO and KIEs were evaluated at both 300 K and 303.15 K (the temperature at which the experimental KIEs were determined).

In step 3, a representative number (Ω) of "snapshot" structures from each of the step 2 MD trajectories were taken in order to re-optimize each to a local stationary point, either an energy minimum or a saddle point. The time separation of these snapshots along each trajectory should be sufficient to ensure statistical independence of the solvent configurations. We chose to select snapshots at 10 ps intervals, thereby obtaining 100 structures for each species. The first solvation shell of DMSO molecules surrounding each solute species was included with the solute in the flexible region for these local relaxations, but the remainder of the solvent was kept frozen in the geometry as found in each individual snapshot from the respective MD trajectory. The reason for this was to generate a set of local stationary points with different solvent configurations representative of the thermal fluctuations occurring at 300 K. Some tests were performed in which the first solvation shell was treated by MM, and the solute by QM, but more generally it was found necessary to treat the first solvation shell and the solute by QM in order to obtain a better description of solute-solvent interactions affecting the KIEs.

The advantage of allowing each snapshot structure to optimize only to a local minimum within a frozen configuration of the environment is that each different structure is more likely to be representative of the whole system at the temperature of the simulation. In contrast, if for each snapshot the whole system is minimised,[24] then the configuration of the environment changes to something corresponding to a much lower temperature and which is unrepresentative of the real system. The method should capture the effects of specific interactions between a substrate and its environment that a continuum model is incapable of doing (for solutes in solution). The sizes of the flexible and frozen regions are a matter of choice, as are the extents of the QM and MM regions and the number of atoms included in the Hessian.

In step 4 a QM/MM Hessian was computed for a subset of atoms from each locally relaxed structure. Usually this subset contained the same atoms as were in the QM region, but sometimes it also included some atoms from the MM region. Any subset of $N_S$ atoms within the environment of a larger $N$-atomic system possesses $3N_S$ vibrational modes, of which $3N_S - 6$ correspond to internal motions within the subset and 6 correspond to motions (librations) of the subset relative to its environment. Although the subset has been relaxed to a local stationary point within a frozen environment, this is not a stationary point within the full system, and the 6 librations are not strictly separable from the $3N_S - 6$ vibrations.

## Conclusion

Ensemble-averaged KIEs take account of multiple configurations in solution at finite temperature, and the methodologies proposed in this study are appropriate for use in situations where specific solute-solvent interactions may be important, which traditional approaches to KIE calculations would neglect. Solvent molecules in the first solvation shell must be included in the Hessian. Provided this is done, then the methods described here and implemented with the hybrid AM1/OPLS-AA potential yield results in (at least) qualitative agreement with experiment, correctly predicting the directions (normal or inverse) of KIEs for six isotopic substitutions.

Although the $\langle KIE \rangle_{\text{indiv}}$ or $\langle KIE \rangle_{\text{state}}$ averaging methods give essentially the same average KIEs, unless one requires to see the distribution of the individual KIE values, for practical purposes we recommend the latter method since it involves less work. We also recommend use of the "all-frequencies" method for evaluation of IPFRs from subset Hessians. The logarithms of the IPFRs for RS and TS do not always show single normal distributions, but appear to reflect different families of solvation configurations. It is not clear whether this is a consequence of the choice of QM method or of inadequate sampling: a more reliable QM method would not necessarily improve either the means or the standard deviations of the average KIEs if the sample of independent solvent configurations is insufficiently representative. How many configurations should be sampled to obtain reliable KIEs? An heuristic approach to answering that important question would be to construct the ln(IPFR) histogram and to update it with each new configuration sampled until the resulting distribution is satisfactory.

Since average KIEs are apparently not very sensitive to the presence of unwanted extra imaginary frequencies, an effective practical procedure might be to sample more snapshot configurations at the expense of less relaxation of the subset atoms to a local stationary point.

The thermally-averaged KIEs may be compared meaningfully with experimental values and the current methodology may perfectly well be implemented with other QM or QM/MM methods, and thus provides a useful tool for investigating KIEs in relation to studies of chemical reaction mechanisms in solution or catalysed by enzymes.

## Acknowledgements

We thank the EPSRC (EP/E019455/1), the Juan de la Cierva subprogramme of the Spanish Ministry of Science (J.J.R.P.) and the General Secretariat of the Spanish Ministry for Education (I.H.W.) for financial support (SAB2010-0116) during sabbatical leave, Prof. Olle Matsson (Uppsala), Dr. Gavin Shaddick (Bath, Statistics), Dr. Ian Greig (Bath) and Prof. Vicente Moliner (Castellon) for helpful discussions, Dr. Giuseppe Ruggiero for some preliminary calculations, and the University of Bath for access to its High Performance Computing Facility.

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## Entry for the Table of Contents

**Better on average**

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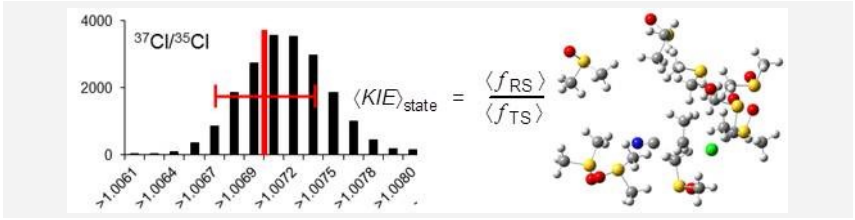
**Ensemble-Averaged QM/MM Kinetic Isotope Effects for the $S_N2$ Reaction of Cyanide Anion with Chloroethane in DMSO Solution**




In contrast to calculations using traditional methods, average AM1/OPLS-AA KIEs computed for $NC^-$ + EtCl in DMSO agree with experiment for isotopic substitutions in six positions, and their distributions for individual configurations provide insight into solvent fluctuation effects. A single-molecule view of chemical change should be replaced by a picture involving averages over representative collections of molecules.

# Ensemble-Average QM/MM Kinetic Isotope Effects for the $S_N2$ Reaction of Cyanide Anion with Chloroethane in DMSO Solution

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## Supporting Information

**Computational Methods**

QM calculations for species in vacuum or in a polarized continuum model[S1] for solution were carried out by means of the Gaussian03[S2] and Gaussian09 programs[S3] with AM1. QM/MM energy minimizations, saddle-point searches and MD calculations, were performed by means of the fDYNAMO library[S4] along with the GRACEFULL interface[S5] to GRACE.[S6] (N.B. the program library GRACE, developed at the University of Bath by Alex J. Turner from 1994 – 1997 and described in his Ph.D. thesis,[S7] should not be confused with the completely separate commercial program of the same name, developed by Marcus A. Neumann of Avant-garde Materials Simulations from 2002 onwards and apparently first reported[S8] in the open literature in 2008.) At each Newton-Raphson step of a QM/MM energy minimization in a control space (the QM subsystem) all geometrical coordinates belonging to the complementary space are minimized. In all cases, the Baker algorithm was employed to localize and characterize the stationary points. All QM/MM minimizations and MD simulations were carried out at 300 K using periodic boundary conditions and Langevin-Verlet NVT conditions, corresponding to the canonical ensemble, in order to keep the number of molecules (and density) constant. A switched cut-off radius of 16.0 Å was employed for all kind of interactions. All atoms of the system were allowed to move, and the time step was 1 fs.

**Preliminaries.** An initial $S_N2$ transition structure was introduced into the center of a pre-equilibrated cubic box (side length 42.5 Å) of explicit DMSO molecules, from which were removed any with a sulfur, oxygen or carbon atom closer than 2.5 Å to any solute atom. The 10 QM atoms of the solute $^{\ddagger}(NC.Et.Cl)^{-}$ were treated by AM1 and the 5390 MM atoms of 539 DMSO molecules were described by OPLS-AA force field potentials.[S9] A similar procedure was followed for both $NC^{-}$ and EtCl individually. Full QM/MM optimization was performed for each of the three species $NC^{-}$, EtCl and $^{\ddagger}(NC.Et.Cl)^{-}$ using the LBFGS method[S10] until the gradient of the energy was converged to < 0.1 kJ $mol^{-1}$. Each solute species in DMSO was then subjected to 500 ps of QM/MM MD at 300 K in order to stabilize and equilibrate the solution; for this purpose the PCM/MP2/6-31+G(d,p) optimized $C_\alpha$-Cl and $C_\alpha$-$C_{nu}$ distances of $^{\ddagger}(NC.Et.Cl)^{-}$ were subjected to harmonic constraints. Finally, an optimized saddle-point structure for $^{\ddagger}(NC.Et.Cl)^{-}$ was obtained.

**Stage 1.** A QM/MM PMF was computed starting from the optimized saddle-point structure for $^{\ddagger}(NC.Et.Cl)^{-}$ and tracing towards both reactants and products using the difference of distances $d(C_\alpha–Cl) - d(C_\alpha–C_{nu})$ as the distinguished coordinate. The initial structure of each window was the final structure of the previous one, and a total of 151 windows were run to

cover the range of interest; in each window a total of 12 ps of QM/MM MD were run: 2 ps relaxation and 10 ps production.

**Stage 2.** A 1 ns QM/MM MD trajectory was computed for the TS, $^{\ddagger}$(NC.Et.Cl)$^{-}$, within the window corresponding to the free energy maximum in the PMF. The distances $C_{\alpha}$–Cl and $C_{\alpha}$–$C_{nu}$ were subjected to an umbrella potential with a force constant of $10^4$ kJ mol$^{-1}$ Å$^{-2}$. In addition, the angle Cl–$C_{\alpha}$–$C_{nu}$ was kept at 180º by means of a harmonic constraint with a very low force constant (5 kJ mol$^{-1}$ Å$^{-2}$): this led to structures being sampled having reasonable orientations of the nucleophile and leaving group, but running the simulation without the angle constraint did not significantly affect the energies and forces. A similar 1 ns QM/MM MD simulation was run without constraints for the apparent "reactant complex" corresponding to the free energy minimum in the PMF, and also for each of the individual reactants $NC^{-}$ and EtCl in its own DMSO box; note the comments above regarding the non-existence of a well-defined precursor ion-molecule complex ($NC^{-}\cdots$EtCl).


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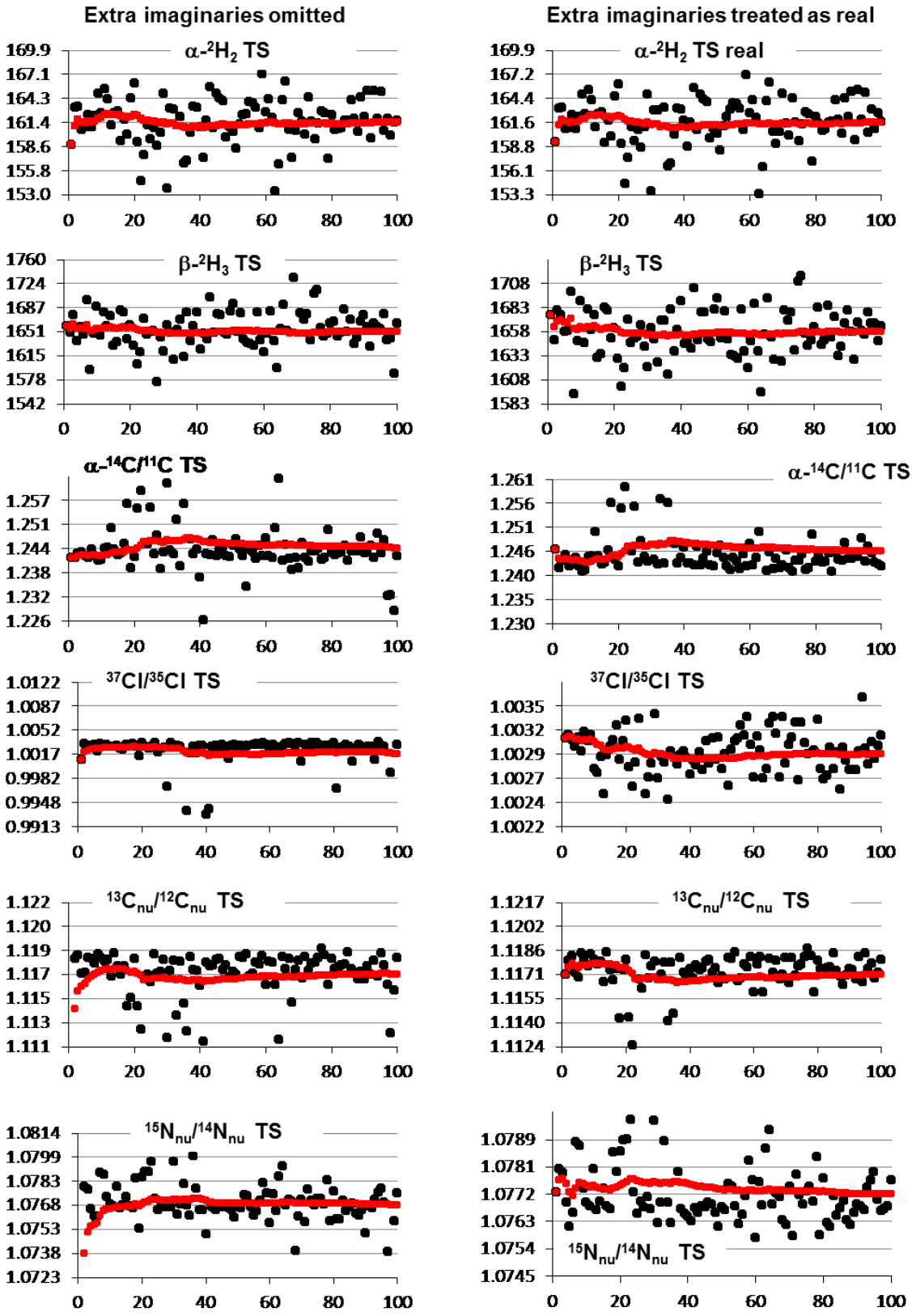


**Figure 4S.** Plots of isotopic partition-function ratios (black dots) against sequence number in the series of locally-relaxed snapshot TS structures for six isotopic substitutions: all IPFRs are computed at 303.15 K by the all-frequencies method, with the left-hand panel showing values obtained by omission of extra imaginary frequencies and the right-hand panel showing values obtained by replacing extra imaginaries by real frequencies of the same magnitude. The red dots show the cumulative mean value of the IPFR up to and including each point in the sequence.

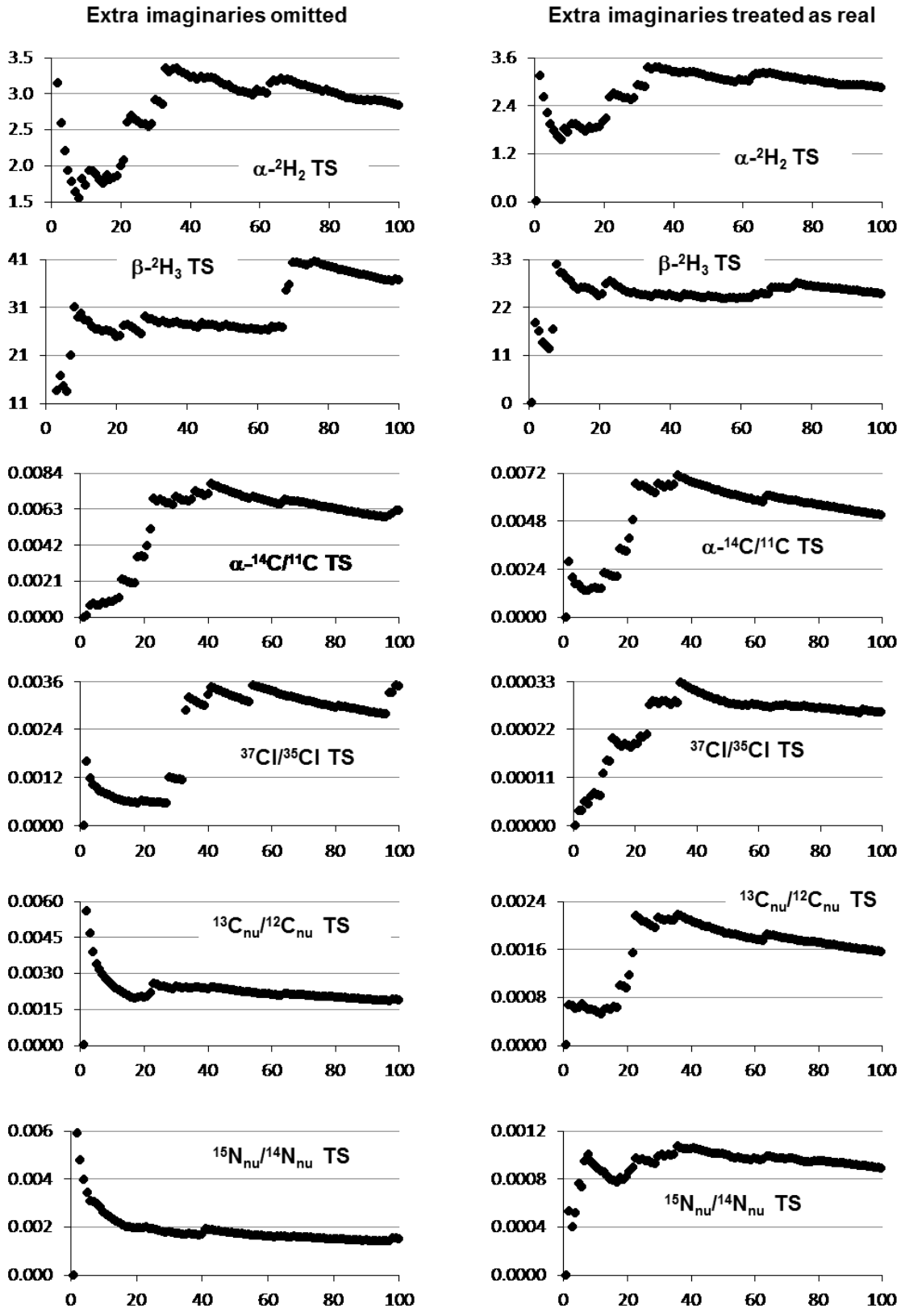


**Figure 5S.** Plots of standard deviation (1σ) corresponding to the cumulative means shown in Fig. S5 isotopic partition-function ratios value of the IPFR up to and including each point in the sequence of locally-relaxed snapshot TS structures for six isotopic substitutions; the left-hand panel is for IPFRs obtained by omission of extra imaginary frequencies and the right-hand panel is for those obtained by replacing extra imaginaries by real frequencies of the same magnitude

## α-$D_2$/α-$H_2$ isotopic partition-function ratios for [NC···Et···Cl]⁻.*n*DMSO transition structures

| structure sequence number | *n* | number extra imaginaries | extra imaginaries treated as reals | | | | extra imaginaries omitted | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | 300 K | | 303.15K | | 300 K | | 303.15K | |
| | | | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ |
| 1 | 8 | 2 | 170.976379 | 170.566264 | 159.410385 | 159.037143 | 170.314285 | 169.905758 | 158.793091 | 158.421294 |
| 2 | 8 | | 175.125015 | 174.768423 | 163.222122 | 162.897784 | 175.125015 | 174.768423 | 163.222122 | 162.897784 |
| 3 | 4 | 1 | 175.230103 | 174.823466 | 163.323746 | 162.953734 | 175.209732 | 174.803143 | 163.304749 | 162.934780 |
| 4 | 5 | 1 | 172.626404 | 172.189622 | 160.926086 | 160.528625 | 172.206863 | 171.771143 | 160.534988 | 160.138493 |
| 5 | 4 | | 172.645538 | 172.272632 | 160.950134 | 160.610807 | 172.645538 | 172.272632 | 160.950134 | 160.610807 |
| 6 | 4 | 1 | 174.354279 | 174.031223 | 162.523483 | 162.229691 | 174.178680 | 173.855950 | 162.359818 | 162.066321 |
| 7 | 4 | | 172.614044 | 172.081115 | 160.912445 | 160.427681 | 172.614044 | 172.081115 | 160.912445 | 160.427681 |
| 8 | 5 | | 174.083710 | 173.670893 | 162.272141 | 161.896609 | 174.083710 | 173.670893 | 162.272141 | 161.896609 |
| 9 | 3 | | 176.882858 | 176.468401 | 164.838501 | 164.461658 | 176.882858 | 176.468401 | 164.838501 | 164.461658 |
| 10 | 4 | | 174.377823 | 173.986967 | 162.544144 | 162.188677 | 174.377823 | 173.986967 | 162.544144 | 162.188677 |
| 11 | 7 | | 177.457306 | 177.030608 | 165.375534 | 164.987557 | 177.457306 | 177.030608 | 165.375534 | 164.987557 |
| 12 | 8 | | 176.150238 | 175.836412 | 164.172531 | 163.887051 | 176.150238 | 175.836412 | 164.172531 | 163.887051 |
| 13 | 8 | | 172.800537 | 172.441293 | 161.087265 | 160.760255 | 172.800537 | 172.441293 | 161.087265 | 160.760255 |
| 14 | 8 | 1 | 174.408630 | 173.964896 | 162.564819 | 162.161150 | 174.352448 | 173.908856 | 162.512436 | 162.108896 |
| 15 | 6 | | 174.648392 | 174.221473 | 162.787445 | 162.399213 | 174.648392 | 174.221473 | 162.787445 | 162.399213 |
| 16 | 6 | | 170.780975 | 170.514205 | 159.224899 | 158.981951 | 170.780975 | 170.514205 | 159.224899 | 158.981951 |
| 17 | 5 | 1 | 173.589691 | 173.074340 | 161.811569 | 161.342759 | 173.583405 | 173.068072 | 161.805710 | 161.336916 |
| 18 | 5 | | 171.606888 | 170.890612 | 159.980713 | 159.330128 | 171.606888 | 170.890612 | 159.980713 | 159.330128 |
| 19 | 5 | 1 | 176.707413 | 176.218574 | 164.664063 | 164.219582 | 176.290909 | 175.803223 | 164.275940 | 163.832507 |
| 20 | 6 | | 178.215515 | 177.705998 | 166.065887 | 165.602954 | 178.215515 | 177.705998 | 166.065887 | 165.602954 |
| 21 | 6 | | 170.741730 | 169.691565 | 159.176559 | 158.224624 | 170.741730 | 169.691565 | 159.176559 | 158.224624 |
| 22 | 8 | | 165.693008 | 164.693194 | 154.524139 | 153.616744 | 165.693008 | 164.693194 | 154.524139 | 153.616744 |
| 23 | 5 | | 168.995422 | 167.903760 | 157.577606 | 156.585604 | 168.995422 | 167.903760 | 157.577606 | 156.585604 |
| 24 | 7 | 1 | 172.798340 | 172.379507 | 161.081421 | 160.700148 | 172.793198 | 172.374378 | 161.076630 | 160.695368 |
| 25 | 3 | | 171.102921 | 170.777740 | 159.522964 | 159.226695 | 171.102921 | 170.777740 | 159.522964 | 159.226695 |
| 26 | 8 | | 172.454620 | 172.218838 | 160.773453 | 160.558855 | 172.454620 | 172.218838 | 160.773453 | 160.558855 |
| 27 | 7 | | 170.201004 | 169.806819 | 158.688461 | 158.329499 | 170.201004 | 169.806819 | 158.688461 | 158.329499 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 28 | 5 | 1 | 172.750534 | 172.197167 | 161.043808 | 160.540775 | 171.899246 | 171.348606 | 160.250229 | 159.749674 |
| 29 | 6 | | 176.928070 | 176.440172 | 164.876221 | 164.432632 | 176.928070 | 176.440172 | 164.876221 | 164.432632 |
| 30 | 7 | | 164.736008 | 163.730804 | 153.643143 | 152.730911 | 164.736008 | 163.730804 | 153.643143 | 152.730911 |
| 31 | 4 | | 174.940460 | 174.709851 | 163.064926 | 162.854938 | 174.940460 | 174.709851 | 163.064926 | 162.854938 |
| 32 | 5 | | 174.914932 | 174.656801 | 163.031494 | 162.796478 | 174.914932 | 174.656801 | 163.031494 | 162.796478 |
| 33 | 5 | 1 | 163.063339 | 162.453500 | 152.107483 | 151.553713 | 161.796280 | 161.191179 | 150.925552 | 150.376085 |
| 34 | 7 | 1 | 175.271011 | 174.972343 | 163.362061 | 163.090287 | 173.888855 | 173.592542 | 162.073837 | 161.804207 |
| 35 | 3 | | 167.959305 | 167.727206 | 156.636551 | 156.424944 | 167.959305 | 167.727206 | 156.636551 | 156.424944 |
| 36 | 5 | | 168.317368 | 167.236145 | 156.959732 | 155.978421 | 168.317368 | 167.236145 | 156.959732 | 155.978421 |
| 37 | 5 | 1 | 171.931580 | 171.589750 | 160.283569 | 159.972302 | 171.878906 | 171.537181 | 160.234451 | 159.923279 |
| 38 | 7 | 1 | 175.197067 | 174.912497 | 163.289841 | 163.030811 | 175.191010 | 174.906449 | 163.284195 | 163.025174 |
| 39 | 9 | | 175.067749 | 174.795118 | 163.172226 | 162.924023 | 175.067749 | 174.795118 | 163.172226 | 162.924023 |
| 40 | 8 | 1 | 173.648987 | 173.193046 | 161.863113 | 161.448210 | 172.652435 | 172.199111 | 160.934189 | 160.521667 |
| 41 | 6 | 2 | 170.366165 | 170.172476 | 158.849304 | 158.672875 | 168.751587 | 168.559733 | 157.343872 | 157.169114 |
| 42 | 5 | | 173.404327 | 173.155671 | 161.650772 | 161.424443 | 173.404327 | 173.155671 | 161.650772 | 161.424443 |
| 43 | 7 | | 177.737335 | 177.314403 | 165.621124 | 165.236579 | 177.737335 | 177.314403 | 165.621124 | 165.236579 |
| 44 | 7 | | 172.477768 | 172.153553 | 160.799332 | 160.504228 | 172.477768 | 172.153553 | 160.799332 | 160.504228 |
| 45 | 4 | | 176.907104 | 176.590907 | 164.868027 | 164.580364 | 176.907104 | 176.590907 | 164.868027 | 164.580364 |
| 46 | 4 | | 176.325287 | 176.007029 | 164.331528 | 164.042000 | 176.325287 | 176.007029 | 164.331528 | 164.042000 |
| 47 | 6 | 2 | 176.009735 | 175.610647 | 164.028976 | 163.665941 | 175.902420 | 175.503575 | 163.928955 | 163.566141 |
| 48 | 6 | | 171.346481 | 171.112337 | 159.753448 | 159.540250 | 171.346481 | 171.112337 | 159.753448 | 159.540250 |
| 49 | 6 | | 172.565109 | 172.371882 | 160.872467 | 160.696456 | 172.565109 | 172.371882 | 160.872467 | 160.696456 |
| 50 | 7 | | 172.013916 | 171.681950 | 160.369720 | 160.067472 | 172.013916 | 171.681950 | 160.369720 | 160.067472 |
| 51 | 6 | | 169.889084 | 169.566606 | 158.410629 | 158.116973 | 169.889084 | 169.566606 | 158.410629 | 158.116973 |
| 52 | 6 | | 172.898209 | 172.522108 | 161.185806 | 160.843734 | 172.898209 | 172.522108 | 161.185806 | 160.843734 |
| 53 | 4 | | 174.120697 | 173.817461 | 162.307953 | 162.031984 | 174.120697 | 173.817461 | 162.307953 | 162.031984 |
| 54 | 6 | 1 | 175.083450 | 174.654696 | 163.183273 | 162.793475 | 174.263962 | 173.837214 | 162.419495 | 162.031521 |
| 55 | 6 | | 175.870377 | 175.507550 | 163.905991 | 163.575897 | 175.870377 | 175.507550 | 163.905991 | 163.575897 |
| 56 | 6 | | 175.697662 | 175.356178 | 163.754471 | 163.443813 | 175.697662 | 175.356178 | 163.754471 | 163.443813 |
| 57 | 7 | | 175.108688 | 174.729794 | 163.202972 | 162.858331 | 175.108688 | 174.729794 | 163.202972 | 162.858331 |
| 58 | 4 | | 172.459396 | 171.777318 | 160.762177 | 160.142066 | 172.459396 | 171.777318 | 160.762177 | 160.142066 |
| 59 | 6 | | 179.343567 | 178.941623 | 167.094101 | 166.728644 | 179.343567 | 178.941623 | 167.094101 | 166.728644 |
| 60 | 7 | | 174.554611 | 174.287908 | 162.690002 | 162.447149 | 174.554611 | 174.287908 | 162.690002 | 162.447149 |
| 61 | 5 | | 176.193390 | 175.821443 | 164.205627 | 163.867384 | 176.193390 | 175.821443 | 164.205627 | 163.867384 |
| 62 | 6 | 1 | 173.953964 | 173.514445 | 162.148544 | 161.748895 | 173.745407 | 173.306415 | 161.954132 | 161.554962 |
| 63 | 6 | | 164.413116 | 163.861036 | 153.351501 | 152.849891 | 164.413116 | 163.861036 | 153.351501 | 152.849891 |
| 64 | 7 | | 167.818466 | 166.747541 | 156.476791 | 155.504814 | 167.818466 | 166.747541 | 156.476791 | 155.504814 |
| 65 | 6 | | 176.088699 | 175.767688 | 164.108994 | 163.816894 | 176.088699 | 175.767688 | 164.108994 | 163.816894 |
| 66 | 4 | | 178.468506 | 177.835795 | 166.292114 | 165.717033 | 178.468506 | 177.835795 | 166.292114 | 165.717033 |
| 67 | 5 | | 172.277603 | 171.828734 | 160.599655 | 160.191446 | 172.277603 | 171.828734 | 160.599655 | 160.191446 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 68 | 7 | 2 | 170.749985 | 170.555798 | 159.196732 | 159.019840 | 168.759201 | 168.567279 | 157.340668 | 157.165839 |
| 69 | 5 | | 172.169525 | 171.983350 | 160.512604 | 160.343004 | 172.169525 | 171.983350 | 160.512604 | 160.343004 |
| 70 | 6 | 1 | 177.020630 | 176.631510 | 164.969040 | 164.615192 | 174.416550 | 174.033154 | 162.542267 | 162.193625 |
| 71 | 7 | | 173.328201 | 172.978440 | 161.571625 | 161.253166 | 173.328201 | 172.978440 | 161.571625 | 161.253166 |
| 72 | 7 | | 171.708298 | 171.334673 | 160.073517 | 159.733643 | 171.708298 | 171.334673 | 160.073517 | 159.733643 |
| 73 | 5 | | 176.452377 | 176.130840 | 164.442322 | 164.149727 | 176.452377 | 176.130840 | 164.442322 | 164.149727 |
| 74 | 3 | | 173.362747 | 173.104561 | 161.602768 | 161.367721 | 173.362747 | 173.104561 | 161.602768 | 161.367721 |
| 75 | 4 | | 171.085510 | 170.733350 | 159.510452 | 159.189914 | 171.085510 | 170.733350 | 159.510452 | 159.189914 |
| 76 | 9 | 1 | 173.119751 | 172.617301 | 161.379211 | 160.922350 | 173.047867 | 172.545625 | 161.312195 | 160.855523 |
| 77 | 7 | | 174.638275 | 174.271078 | 162.779068 | 162.445131 | 174.638275 | 174.271078 | 162.779068 | 162.445131 |
| 78 | 7 | | 174.422928 | 174.033790 | 162.582520 | 162.228703 | 174.422928 | 174.033790 | 162.582520 | 162.228703 |
| 79 | 9 | | 168.542419 | 168.275841 | 157.156845 | 156.913998 | 168.542419 | 168.275841 | 157.156845 | 156.913998 |
| 80 | 7 | | 174.098602 | 173.544518 | 162.276871 | 161.773168 | 174.098602 | 173.544518 | 162.276871 | 161.773168 |
| 81 | 8 | 1 | 173.243668 | 172.837985 | 161.496964 | 161.127846 | 172.204453 | 171.801203 | 160.528259 | 160.161356 |
| 82 | 6 | 1 | 172.376465 | 172.135385 | 160.704544 | 160.485114 | 172.359573 | 172.118518 | 160.688812 | 160.469404 |
| 83 | 10 | | 172.524277 | 172.249015 | 160.837158 | 160.586602 | 172.524277 | 172.249015 | 160.837158 | 160.586602 |
| 84 | 6 | | 173.448669 | 172.985387 | 161.678055 | 161.256678 | 173.448669 | 172.985387 | 161.678055 | 161.256678 |
| 85 | 6 | | 173.475204 | 173.179369 | 161.710129 | 161.440959 | 173.475204 | 173.179369 | 161.710129 | 161.440959 |
| 86 | 6 | 1 | 176.181778 | 175.585412 | 164.191742 | 163.649604 | 176.014160 | 175.418361 | 164.035522 | 163.493900 |
| 87 | 8 | | 173.689194 | 173.399319 | 161.907104 | 161.643214 | 173.689194 | 173.399319 | 161.907104 | 161.643214 |
| 88 | 7 | | 171.953644 | 171.791286 | 160.310959 | 160.163014 | 171.953644 | 171.791286 | 160.310959 | 160.163014 |
| 89 | 8 | | 176.379501 | 175.939089 | 164.376846 | 163.976153 | 176.379501 | 175.939089 | 164.376846 | 163.976153 |
| 90 | 7 | 1 | 174.066742 | 173.718042 | 162.253021 | 161.935724 | 173.969101 | 173.620597 | 162.162003 | 161.844884 |
| 91 | 8 | | 177.180359 | 176.837261 | 165.119308 | 164.807134 | 177.180359 | 176.837261 | 165.119308 | 164.807134 |
| 92 | 7 | 1 | 171.197342 | 170.919115 | 159.606354 | 159.352996 | 171.196884 | 170.918658 | 159.605942 | 159.352585 |
| 93 | 6 | 2 | 177.526825 | 177.139503 | 165.428223 | 165.076013 | 177.270920 | 176.884156 | 165.189758 | 164.838056 |
| 94 | 7 | | 173.703018 | 173.215358 | 161.912750 | 161.469105 | 173.703018 | 173.215358 | 161.912750 | 161.469105 |
| 95 | 7 | | 177.137070 | 176.645924 | 165.071518 | 164.625023 | 177.137070 | 176.645924 | 165.071518 | 164.625023 |
| 96 | 7 | | 172.118973 | 171.721577 | 160.463623 | 160.101898 | 172.118973 | 171.721577 | 160.463623 | 160.101898 |
| 97 | 9 | 4 | 174.973175 | 174.555725 | 163.083862 | 162.703983 | 173.637192 | 173.222929 | 161.838684 | 161.461705 |
| 98 | 7 | 1 | 172.534637 | 172.288401 | 160.839203 | 160.614930 | 171.531693 | 171.286887 | 159.904236 | 159.681267 |
| 99 | 5 | 1 | 174.603210 | 174.329211 | 162.739029 | 162.489622 | 173.182571 | 172.910801 | 161.414948 | 161.167570 |
| 100 | 7 | | 173.451782 | 173.075408 | 161.685989 | 161.343578 | 173.451782 | 173.075408 | 161.685989 | 161.343578 |

## β-$D_3$/β-$H_3$ isotopic partition-function ratios for [NC···Et···Cl]$^-$.*n*DMSO transition structures

| structure sequence number | *n* | number extra imaginaries | extra imaginaries treated as reals | | | | extra imaginaries omitted | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | 300 K | | 303.15K | | 300 K | | 303.15K | |
| | | | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ |
| 1 | 8 | 2 | 1853.868652 | 1839.330275 | 1675.373047 | 1662.547026 | 1822.517608 | 1808.225092 | 1660.059204 | 1647.350421 |
| 2 | 8 | | 1825.052124 | 1809.766027 | 1649.608521 | 1636.123535 | 1809.766027 | 1794.607962 | 1649.608521 | 1636.123535 |
| 3 | 4 | 1 | 1858.934326 | 1844.431124 | 1679.807739 | 1667.011948 | 1840.383726 | 1826.025254 | 1676.121582 | 1663.353870 |
| 4 | 5 | 1 | 1853.907715 | 1839.555337 | 1675.387451 | 1662.725492 | 1797.475687 | 1783.560188 | 1637.063354 | 1624.691035 |
| 5 | 4 | | 1834.571045 | 1820.629490 | 1657.977539 | 1645.678206 | 1820.629490 | 1806.793883 | 1657.977539 | 1645.678206 |
| 6 | 4 | 1 | 1836.002197 | 1819.642104 | 1659.392944 | 1644.965205 | 1806.361120 | 1790.265150 | 1647.281738 | 1632.959300 |
| 7 | 4 | | 1880.895752 | 1865.503817 | 1699.412476 | 1685.841357 | 1865.503817 | 1850.237838 | 1699.412476 | 1685.841357 |
| 8 | 5 | | 1762.019897 | 1747.938938 | 1593.240845 | 1580.814068 | 1747.938938 | 1733.970505 | 1593.240845 | 1580.814068 |
| 9 | 3 | | 1824.000732 | 1808.507417 | 1648.757813 | 1635.092079 | 1808.507417 | 1793.145704 | 1648.757813 | 1635.092079 |
| 10 | 4 | | 1869.625977 | 1853.621083 | 1689.295654 | 1675.184876 | 1853.621083 | 1837.753199 | 1689.295654 | 1675.184876 |
| 11 | 7 | | 1821.012451 | 1805.638081 | 1646.105713 | 1632.544771 | 1805.638081 | 1790.393513 | 1646.105713 | 1632.544771 |
| 12 | 8 | | 1860.274170 | 1845.189034 | 1681.098022 | 1667.791296 | 1845.189034 | 1830.226225 | 1681.098022 | 1667.791296 |
| 13 | 8 | | 1836.559570 | 1822.048123 | 1660.008423 | 1647.199303 | 1822.048123 | 1807.651337 | 1660.008423 | 1647.199303 |
| 14 | 8 | 1 | 1853.515625 | 1838.326427 | 1675.108276 | 1661.709280 | 1837.690447 | 1822.630933 | 1674.528687 | 1661.134326 |
| 15 | 6 | | 1803.705811 | 1788.278987 | 1630.600708 | 1616.992749 | 1788.278987 | 1772.984106 | 1630.600708 | 1616.992749 |
| 16 | 6 | | 1808.643311 | 1796.528995 | 1635.058716 | 1624.360071 | 1796.528995 | 1784.495822 | 1635.058716 | 1624.360071 |
| 17 | 5 | 1 | 1862.759644 | 1847.301613 | 1683.354370 | 1669.720148 | 1846.921130 | 1831.594535 | 1683.007690 | 1669.376276 |
| 18 | 5 | | 1859.707520 | 1841.487343 | 1680.381592 | 1664.339598 | 1841.487343 | 1823.445675 | 1680.381592 | 1664.339598 |
| 19 | 5 | 1 | 1826.318237 | 1811.438894 | 1650.865112 | 1637.739738 | 1800.005344 | 1785.340377 | 1640.445190 | 1627.402660 |
| 20 | 6 | | 1838.177246 | 1821.175777 | 1661.404053 | 1646.419326 | 1821.175777 | 1804.331557 | 1661.404053 | 1646.419326 |
| 21 | 6 | | 1803.267578 | 1782.991209 | 1630.271484 | 1612.445715 | 1782.991209 | 1762.942833 | 1630.271484 | 1612.445715 |
| 22 | 8 | | 1770.656250 | 1752.671186 | 1601.185425 | 1585.356827 | 1752.671186 | 1734.868802 | 1601.185425 | 1585.356827 |
| 23 | 5 | | 1791.895264 | 1776.380088 | 1620.162109 | 1606.490134 | 1776.380088 | 1760.999251 | 1620.162109 | 1606.490134 |
| 24 | 7 | 1 | 1848.780518 | 1834.917652 | 1670.841675 | 1658.605957 | 1834.356099 | 1820.601393 | 1670.330322 | 1658.098349 |
| 25 | 3 | | 1821.526367 | 1809.237601 | 1646.566162 | 1635.709879 | 1809.237601 | 1797.031740 | 1646.566162 | 1635.709879 |
| 26 | 8 | | 1827.344604 | 1812.803477 | 1651.599976 | 1638.767828 | 1812.803477 | 1798.378060 | 1651.599976 | 1638.767828 |

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|---|---|---|---|---|---|---|---|---|---|---|
| 27 | 7 | | 1828.554565 | 1815.415888 | 1652.708618 | 1641.108875 | 1815.415888 | 1802.371616 | 1652.708618 | 1641.108875 |
| 28 | 5 | 1 | 1841.737793 | 1825.410351 | 1664.501831 | 1650.111224 | 1727.048574 | 1711.737878 | 1574.811768 | 1561.196584 |
| 29 | 6 | | 1817.357056 | 1801.602137 | 1642.696899 | 1628.801372 | 1801.602137 | 1785.983799 | 1642.696899 | 1628.801372 |
| 30 | 7 | | 1793.787842 | 1775.259793 | 1621.763916 | 1605.463064 | 1775.259793 | 1756.923120 | 1621.763916 | 1605.463064 |
| 31 | 4 | | 1838.546021 | 1825.992958 | 1661.661865 | 1650.577593 | 1825.992958 | 1813.525603 | 1661.661865 | 1650.577593 |
| 32 | 5 | | 1825.256226 | 1812.823820 | 1649.862793 | 1638.884370 | 1812.823820 | 1800.476095 | 1649.862793 | 1638.884370 |
| 33 | 5 | 1 | 1798.429810 | 1777.612800 | 1625.807861 | 1607.485319 | 1759.604451 | 1739.236849 | 1609.337402 | 1591.200479 |
| 34 | 7 | 1 | 1847.291016 | 1832.882287 | 1669.563843 | 1656.848870 | 1815.327904 | 1801.168485 | 1653.573730 | 1640.980534 |
| 35 | 3 | | 1847.403931 | 1837.326861 | 1669.570068 | 1660.666440 | 1837.326861 | 1827.304759 | 1669.570068 | 1660.666440 |
| 36 | 5 | | 1784.420166 | 1766.677023 | 1613.259521 | 1597.645809 | 1766.677023 | 1749.110307 | 1613.259521 | 1597.645809 |
| 37 | 5 | 1 | 1859.815674 | 1846.229118 | 1680.655884 | 1668.662444 | 1846.109393 | 1832.622966 | 1680.546997 | 1668.554335 |
| 38 | 7 | 1 | 1811.705078 | 1798.664792 | 1637.736328 | 1626.222537 | 1797.906132 | 1784.965168 | 1637.045654 | 1625.536719 |
| 39 | 9 | | 1836.901611 | 1823.922700 | 1660.158447 | 1648.699969 | 1823.922700 | 1811.035494 | 1660.158447 | 1648.699969 |
| 40 | 8 | 1 | 1870.512573 | 1856.429446 | 1689.917114 | 1677.494565 | 1846.038546 | 1832.139685 | 1680.458374 | 1668.105356 |
| 41 | 6 | 2 | 1819.924438 | 1807.840435 | 1645.167236 | 1634.494429 | 1784.972416 | 1773.120487 | 1624.357056 | 1613.819251 |
| 42 | 5 | | 1823.442993 | 1809.356678 | 1648.307007 | 1635.872800 | 1809.356678 | 1795.379181 | 1648.307007 | 1635.872800 |
| 43 | 7 | | 1814.677246 | 1799.369018 | 1640.479858 | 1626.975041 | 1799.369018 | 1784.189926 | 1640.479858 | 1626.975041 |
| 44 | 7 | | 1885.237427 | 1870.583735 | 1703.374268 | 1690.446273 | 1870.583735 | 1856.043944 | 1703.374268 | 1690.446273 |
| 45 | 4 | | 1824.626221 | 1810.652354 | 1649.220581 | 1636.889284 | 1810.652354 | 1796.785507 | 1649.220581 | 1636.889284 |
| 46 | 4 | | 1857.172974 | 1842.304711 | 1678.388550 | 1665.270937 | 1842.304711 | 1827.555482 | 1678.388550 | 1665.270937 |
| 47 | 6 | 2 | 1856.364136 | 1841.067945 | 1677.685425 | 1664.190616 | 1840.394706 | 1825.230101 | 1677.072021 | 1663.582147 |
| 48 | 6 | | 1825.644287 | 1812.473636 | 1650.212036 | 1638.583881 | 1812.473636 | 1799.398001 | 1650.212036 | 1638.583881 |
| 49 | 6 | | 1822.324585 | 1810.844642 | 1647.309570 | 1637.168688 | 1810.844642 | 1799.437018 | 1647.309570 | 1637.168688 |
| 50 | 7 | | 1860.754761 | 1847.008622 | 1681.486572 | 1669.354107 | 1847.008622 | 1833.364031 | 1681.486572 | 1669.354107 |
| 51 | 6 | | 1873.565308 | 1859.451603 | 1692.929810 | 1680.473914 | 1859.451603 | 1845.444217 | 1692.929810 | 1680.473914 |
| 52 | 6 | | 1826.689819 | 1811.641625 | 1650.825439 | 1637.556327 | 1811.641625 | 1796.717398 | 1650.825439 | 1637.556327 |
| 53 | 4 | | 1857.562988 | 1843.712437 | 1678.694824 | 1666.473039 | 1843.712437 | 1829.965159 | 1678.694824 | 1666.473039 |
| 54 | 6 | 1 | 1825.743408 | 1809.695094 | 1650.235718 | 1636.084516 | 1797.947344 | 1782.143358 | 1639.523193 | 1625.463855 |
| 55 | 6 | | 1807.817383 | 1794.116530 | 1634.389160 | 1622.296375 | 1794.116530 | 1780.519511 | 1634.389160 | 1622.296375 |
| 56 | 6 | | 1806.513306 | 1792.414672 | 1633.203369 | 1620.760831 | 1792.414672 | 1778.426069 | 1633.203369 | 1620.760831 |
| 57 | 7 | | 1802.959106 | 1788.724757 | 1629.903931 | 1617.343816 | 1788.724757 | 1774.602788 | 1629.903931 | 1617.343816 |
| 58 | 4 | | 1860.542603 | 1844.248065 | 1681.302246 | 1666.939959 | 1844.248065 | 1828.096235 | 1681.302246 | 1666.939959 |
| 59 | 6 | | 1811.786011 | 1796.866641 | 1637.916992 | 1624.753491 | 1796.866641 | 1782.070127 | 1637.916992 | 1624.753491 |
| 60 | 7 | | 1792.515381 | 1781.238610 | 1620.707031 | 1610.745081 | 1781.238610 | 1770.032781 | 1620.707031 | 1610.745081 |
| 61 | 5 | | 1823.040039 | 1807.712552 | 1647.937866 | 1634.416640 | 1807.712552 | 1792.513933 | 1647.937866 | 1634.416640 |
| 62 | 6 | 1 | 1866.385742 | 1850.693486 | 1686.472290 | 1672.638711 | 1845.946263 | 1830.425858 | 1682.146240 | 1668.348146 |
| 63 | 6 | | 1811.379517 | 1792.788634 | 1637.454712 | 1621.081742 | 1792.788634 | 1774.388557 | 1637.454712 | 1621.081742 |
| 64 | 7 | | 1764.297363 | 1746.875453 | 1595.574707 | 1580.237149 | 1746.875453 | 1729.625580 | 1595.574707 | 1580.237149 |
| 65 | 6 | | 1831.330200 | 1817.594364 | 1655.191528 | 1643.069234 | 1817.594364 | 1803.961552 | 1655.191528 | 1643.069234 |
| 66 | 4 | | 1873.240356 | 1857.580684 | 1692.517456 | 1678.714290 | 1857.580684 | 1842.051921 | 1692.517456 | 1678.714290 |

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|---|---|---|---|---|---|---|---|---|---|---|
| 67 | 5 | | 1828.127930 | 1812.675833 | 1652.420532 | 1638.793877 | 1812.675833 | 1797.354344 | 1652.420532 | 1638.793877 |
| 68 | 7 | 2 | 1801.812012 | 1790.752227 | 1628.946899 | 1619.176839 | 1616.401051 | 1606.479345 | 1470.351685 | 1461.532843 |
| 69 | 5 | | 1918.717041 | 1907.262527 | 1733.101807 | 1722.991229 | 1907.262527 | 1895.876394 | 1733.101807 | 1722.991229 |
| 70 | 6 | 1 | 1799.353027 | 1784.075723 | 1626.775635 | 1613.296658 | 1632.170818 | 1618.312965 | 1488.264893 | 1475.933574 |
| 71 | 7 | | 1858.578003 | 1845.006138 | 1679.595947 | 1667.615177 | 1845.006138 | 1831.533379 | 1679.595947 | 1667.615177 |
| 72 | 7 | | 1846.841187 | 1831.376554 | 1669.026367 | 1655.387821 | 1831.376554 | 1816.041415 | 1669.026367 | 1655.387821 |
| 73 | 5 | | 1857.603516 | 1844.156243 | 1678.547363 | 1666.681126 | 1844.156243 | 1830.806315 | 1678.547363 | 1666.681126 |
| 74 | 3 | | 1812.998047 | 1799.895395 | 1638.994751 | 1627.425611 | 1799.895395 | 1786.887438 | 1638.994751 | 1627.425611 |
| 75 | 4 | | 1892.354980 | 1877.505086 | 1709.625244 | 1696.526404 | 1877.505086 | 1862.771723 | 1709.625244 | 1696.526404 |
| 76 | 9 | 1 | 1898.959351 | 1882.744776 | 1715.455933 | 1701.166922 | 1882.456366 | 1866.382705 | 1715.193237 | 1700.906415 |
| 77 | 7 | | 1832.332520 | 1816.949403 | 1656.131104 | 1642.564073 | 1816.949403 | 1801.695434 | 1656.131104 | 1642.564073 |
| 78 | 7 | | 1818.299072 | 1802.418937 | 1643.678711 | 1629.674165 | 1802.418937 | 1786.677492 | 1643.678711 | 1629.674165 |
| 79 | 9 | | 1824.514404 | 1811.949701 | 1648.956665 | 1637.861316 | 1811.949701 | 1799.471525 | 1648.956665 | 1637.861316 |
| 80 | 7 | | 1840.589478 | 1825.412846 | 1663.223267 | 1649.846671 | 1825.412846 | 1810.361354 | 1663.223267 | 1649.846671 |
| 81 | 8 | 1 | 1861.950806 | 1847.056390 | 1682.558716 | 1669.420245 | 1829.299554 | 1814.666327 | 1666.383789 | 1653.371622 |
| 82 | 6 | 1 | 1819.456177 | 1805.737717 | 1644.638794 | 1632.530656 | 1805.614023 | 1791.999930 | 1644.526123 | 1632.418814 |
| 83 | 10 | | 1824.613892 | 1810.962145 | 1649.189575 | 1637.140531 | 1810.962145 | 1797.412540 | 1649.189575 | 1637.140531 |
| 84 | 6 | | 1864.977417 | 1849.092687 | 1685.279175 | 1671.271257 | 1849.092687 | 1833.343254 | 1685.279175 | 1671.271257 |
| 85 | 6 | | 1827.629272 | 1813.132286 | 1651.829346 | 1639.039229 | 1813.132286 | 1798.750291 | 1651.829346 | 1639.039229 |
| 86 | 6 | 1 | 1851.513428 | 1835.748783 | 1673.172485 | 1659.274671 | 1831.423379 | 1815.829791 | 1669.230103 | 1655.365035 |
| 87 | 8 | | 1805.885498 | 1793.302587 | 1632.536743 | 1621.427034 | 1793.302587 | 1780.807351 | 1632.536743 | 1621.427034 |
| 88 | 7 | | 1816.932495 | 1806.703677 | 1642.396851 | 1633.359134 | 1806.703677 | 1796.532444 | 1642.396851 | 1633.359134 |
| 89 | 8 | | 1843.844971 | 1829.246725 | 1666.447266 | 1653.565616 | 1829.246725 | 1814.764057 | 1666.447266 | 1653.565616 |
| 90 | 7 | 1 | 1859.041016 | 1845.133790 | 1679.840210 | 1667.571637 | 1842.197669 | 1828.416446 | 1677.167236 | 1664.918185 |
| 91 | 8 | | 1834.617554 | 1820.865152 | 1658.278076 | 1646.140590 | 1820.865152 | 1807.215840 | 1658.278076 | 1646.140590 |
| 92 | 7 | 1 | 1801.847290 | 1789.316144 | 1628.952759 | 1617.886761 | 1789.302568 | 1776.858665 | 1628.940430 | 1617.874516 |
| 93 | 6 | 2 | 1845.433472 | 1829.911109 | 1667.642944 | 1653.953280 | 1826.230658 | 1810.869815 | 1664.288940 | 1650.626809 |
| 94 | 7 | | 1834.956543 | 1820.603008 | 1658.564209 | 1645.900680 | 1820.603008 | 1806.361750 | 1658.564209 | 1645.900680 |
| 95 | 7 | | 1831.290283 | 1815.513031 | 1655.152100 | 1641.239806 | 1815.513031 | 1799.871707 | 1655.152100 | 1641.239806 |
| 96 | 7 | | 1856.586670 | 1842.393487 | 1677.690186 | 1665.166620 | 1842.393487 | 1828.308808 | 1677.690186 | 1665.166620 |
| 97 | 9 | 4 | 1844.624512 | 1829.887056 | 1667.017822 | 1654.013224 | 1798.885636 | 1784.513607 | 1638.775879 | 1625.991599 |
| 98 | 7 | 1 | 1844.124878 | 1832.547612 | 1666.604614 | 1656.381408 | 1803.933341 | 1792.608394 | 1640.581543 | 1630.517966 |
| 99 | 5 | 1 | 1823.596924 | 1811.079517 | 1648.326782 | 1637.275953 | 1745.103144 | 1733.124528 | 1588.279541 | 1577.631285 |
| 100 | 7 | | 1840.478394 | 1825.479187 | 1663.388916 | 1650.157525 | 1825.479187 | 1810.602218 | 1663.388916 | 1650.157525 |

## $\alpha$-$^{14}$C/$\alpha$-$^{11}$C isotopic partition-function ratios for [NC···Et···Cl]$^{-}$.*n*DMSO transition structures

| structure sequence number | *n* | number extra imaginaries | extra imaginaries treated as reals | | | | extra imaginaries omitted | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | 300 K | | 303.15K | | 300 K | | 303.15K | |
| | | | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ |
| 1 | 8 | 2 | 1.251411 | 1.175983 | 1.245848 | 1.172492 | 1.247621 | 1.172421 | 1.242075 | 1.168941 |
| 2 | 8 | | 1.247473 | 1.165087 | 1.241926 | 1.161815 | 1.247473 | 1.165087 | 1.241926 | 1.161815 |
| 3 | 4 | 1 | 1.249057 | 1.175234 | 1.243493 | 1.171689 | 1.248776 | 1.174969 | 1.243213 | 1.171425 |
| 4 | 5 | 1 | 1.250206 | 1.174806 | 1.244664 | 1.171333 | 1.249062 | 1.173731 | 1.243525 | 1.170261 |
| 5 | 4 | | 1.247968 | 1.170468 | 1.242441 | 1.167069 | 1.247968 | 1.170468 | 1.242441 | 1.167069 |
| 6 | 4 | 1 | 1.248983 | 1.161574 | 1.243420 | 1.158442 | 1.247495 | 1.160190 | 1.241938 | 1.157061 |
| 7 | 4 | | 1.249643 | 1.166068 | 1.244098 | 1.162840 | 1.249643 | 1.166068 | 1.244098 | 1.162840 |
| 8 | 5 | | 1.247972 | 1.166789 | 1.242435 | 1.163491 | 1.247972 | 1.166789 | 1.242435 | 1.163491 |
| 9 | 3 | | 1.246808 | 1.159597 | 1.241258 | 1.156468 | 1.246808 | 1.159597 | 1.241258 | 1.156468 |
| 10 | 4 | | 1.247070 | 1.159982 | 1.241538 | 1.156868 | 1.247070 | 1.159982 | 1.241538 | 1.156868 |
| 11 | 7 | | 1.249913 | 1.163629 | 1.244342 | 1.160457 | 1.249913 | 1.163629 | 1.244342 | 1.160457 |
| 12 | 8 | | 1.250162 | 1.171912 | 1.244596 | 1.168501 | 1.250162 | 1.171912 | 1.244596 | 1.168501 |
| 13 | 8 | | 1.255299 | 1.188679 | 1.249702 | 1.184896 | 1.255299 | 1.188679 | 1.249702 | 1.184896 |
| 14 | 8 | 1 | 1.250172 | 1.171211 | 1.244612 | 1.167828 | 1.249684 | 1.170754 | 1.244127 | 1.167372 |
| 15 | 6 | | 1.248381 | 1.161157 | 1.242835 | 1.158037 | 1.248381 | 1.161157 | 1.242835 | 1.158037 |
| 16 | 6 | | 1.248705 | 1.187464 | 1.243174 | 1.183581 | 1.248705 | 1.187464 | 1.243174 | 1.183581 |
| 17 | 5 | 1 | 1.251257 | 1.171399 | 1.245692 | 1.168040 | 1.251238 | 1.171381 | 1.245673 | 1.168022 |
| 18 | 5 | | 1.261466 | 1.156054 | 1.255807 | 1.153447 | 1.261466 | 1.156054 | 1.255807 | 1.153447 |
| 19 | 5 | 1 | 1.249245 | 1.165089 | 1.243686 | 1.161863 | 1.244971 | 1.161104 | 1.239431 | 1.157888 |
| 20 | 6 | | 1.247903 | 1.148239 | 1.242344 | 1.145495 | 1.247903 | 1.148239 | 1.242344 | 1.145495 |
| 21 | 6 | | 1.260334 | 1.122619 | 1.254692 | 1.121172 | 1.260334 | 1.122619 | 1.254692 | 1.121172 |
| 22 | 8 | | 1.264832 | 1.144383 | 1.259162 | 1.142313 | 1.264832 | 1.144383 | 1.259162 | 1.142313 |
| 23 | 5 | | 1.273493 | 1.182393 | 1.267786 | 1.179320 | 1.273493 | 1.182393 | 1.267786 | 1.179320 |
| 24 | 7 | 1 | 1.251180 | 1.183872 | 1.245593 | 1.180113 | 1.251166 | 1.183859 | 1.245578 | 1.180100 |
| 25 | 3 | | 1.260697 | 1.211687 | 1.255045 | 1.207344 | 1.260697 | 1.211687 | 1.255045 | 1.207344 |
| 26 | 8 | | 1.248610 | 1.175194 | 1.243072 | 1.171662 | 1.248610 | 1.175194 | 1.243072 | 1.171662 |

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|---|---|---|---|---|---|---|---|---|---|---|
| 27 | 7 | | 1.253300 | 1.191661 | 1.247737 | 1.187763 | 1.253300 | 1.191661 | 1.247737 | 1.187763 |
| 28 | 5 | 1 | 1.249796 | 1.153957 | 1.244255 | 1.151119 | 1.244544 | 1.149108 | 1.239027 | 1.146282 |
| 29 | 6 | | 1.248988 | 1.162333 | 1.243426 | 1.159181 | 1.248988 | 1.162333 | 1.243426 | 1.159181 |
| 30 | 7 | | 1.266845 | 1.145662 | 1.261152 | 1.143608 | 1.266845 | 1.145662 | 1.261152 | 1.143608 |
| 31 | 4 | | 1.249392 | 1.189925 | 1.243848 | 1.185978 | 1.249392 | 1.189925 | 1.243848 | 1.185978 |
| 32 | 5 | | 1.248379 | 1.187381 | 1.242845 | 1.183488 | 1.248379 | 1.187381 | 1.242845 | 1.183488 |
| 33 | 5 | 1 | 1.262194 | 1.144193 | 1.256524 | 1.142015 | 1.257573 | 1.140004 | 1.251924 | 1.137834 |
| 34 | 7 | 1 | 1.248456 | 1.175145 | 1.242911 | 1.171602 | 1.245411 | 1.172279 | 1.239879 | 1.168745 |
| 35 | 3 | | 1.261466 | 1.221306 | 1.255834 | 1.216734 | 1.261466 | 1.221306 | 1.255834 | 1.216734 |
| 36 | 5 | | 1.269416 | 1.153560 | 1.263707 | 1.151311 | 1.269416 | 1.153560 | 1.263707 | 1.151311 |
| 37 | 5 | 1 | 1.252769 | 1.191210 | 1.247186 | 1.187290 | 1.252472 | 1.190927 | 1.246890 | 1.187007 |
| 38 | 7 | 1 | 1.248515 | 1.182687 | 1.242967 | 1.178920 | 1.248449 | 1.182625 | 1.242901 | 1.178858 |
| 39 | 9 | | 1.249615 | 1.187036 | 1.244054 | 1.183164 | 1.249615 | 1.187036 | 1.244054 | 1.183164 |
| 40 | 8 | 1 | 1.251817 | 1.179393 | 1.246246 | 1.175803 | 1.242514 | 1.170628 | 1.236984 | 1.167065 |
| 41 | 6 | 2 | 1.248453 | 1.189918 | 1.242919 | 1.185954 | 1.231533 | 1.173791 | 1.226074 | 1.169881 |
| 42 | 5 | | 1.248475 | 1.177343 | 1.242917 | 1.173722 | 1.248475 | 1.177343 | 1.242917 | 1.173722 |
| 43 | 7 | | 1.248185 | 1.163240 | 1.242632 | 1.160041 | 1.248185 | 1.163240 | 1.242632 | 1.160041 |
| 44 | 7 | | 1.252037 | 1.181049 | 1.246466 | 1.177416 | 1.252037 | 1.181049 | 1.246466 | 1.177416 |
| 45 | 4 | | 1.248096 | 1.172660 | 1.242535 | 1.169164 | 1.248096 | 1.172660 | 1.242535 | 1.169164 |
| 46 | 4 | | 1.249525 | 1.173181 | 1.243966 | 1.169717 | 1.249525 | 1.173181 | 1.243966 | 1.169717 |
| 47 | 6 | 2 | 1.251119 | 1.174376 | 1.245535 | 1.170903 | 1.250534 | 1.173827 | 1.244953 | 1.170356 |
| 48 | 6 | | 1.248034 | 1.182909 | 1.242509 | 1.179144 | 1.248034 | 1.182909 | 1.242509 | 1.179144 |
| 49 | 6 | | 1.247830 | 1.193131 | 1.242302 | 1.189062 | 1.247830 | 1.193131 | 1.242302 | 1.189062 |
| 50 | 7 | | 1.250690 | 1.185205 | 1.245133 | 1.181421 | 1.250690 | 1.185205 | 1.245133 | 1.181421 |
| 51 | 6 | | 1.252356 | 1.188191 | 1.246793 | 1.184366 | 1.252356 | 1.188191 | 1.246793 | 1.184366 |
| 52 | 6 | | 1.249741 | 1.162763 | 1.244185 | 1.159628 | 1.249741 | 1.162763 | 1.244185 | 1.159628 |
| 53 | 4 | | 1.247899 | 1.175580 | 1.242366 | 1.172020 | 1.247899 | 1.175580 | 1.242366 | 1.172020 |
| 54 | 6 | 1 | 1.247155 | 1.155601 | 1.241609 | 1.152613 | 1.239996 | 1.148968 | 1.234482 | 1.145997 |
| 55 | 6 | | 1.249677 | 1.174984 | 1.244124 | 1.171478 | 1.249677 | 1.174984 | 1.244124 | 1.171478 |
| 56 | 6 | | 1.248876 | 1.171553 | 1.243334 | 1.168134 | 1.248876 | 1.171553 | 1.243334 | 1.168134 |
| 57 | 7 | | 1.247214 | 1.167381 | 1.241693 | 1.164060 | 1.247214 | 1.167381 | 1.241693 | 1.164060 |
| 58 | 4 | | 1.250603 | 1.157271 | 1.245037 | 1.154327 | 1.250603 | 1.157271 | 1.245037 | 1.154327 |
| 59 | 6 | | 1.248023 | 1.164925 | 1.242461 | 1.161660 | 1.248023 | 1.164925 | 1.242461 | 1.161660 |
| 60 | 7 | | 1.252591 | 1.196293 | 1.247024 | 1.192236 | 1.252591 | 1.196293 | 1.247024 | 1.192236 |
| 61 | 5 | | 1.248041 | 1.163652 | 1.242487 | 1.160436 | 1.248041 | 1.163652 | 1.242487 | 1.160436 |
| 62 | 6 | 1 | 1.249702 | 1.160058 | 1.244135 | 1.156995 | 1.247579 | 1.158087 | 1.242021 | 1.155028 |
| 63 | 6 | | 1.255303 | 1.145493 | 1.249723 | 1.143101 | 1.255303 | 1.145493 | 1.249723 | 1.143101 |
| 64 | 7 | | 1.268133 | 1.152982 | 1.262422 | 1.150699 | 1.268133 | 1.152982 | 1.262422 | 1.150699 |
| 65 | 6 | | 1.246910 | 1.174496 | 1.241372 | 1.170932 | 1.246910 | 1.174496 | 1.241372 | 1.170932 |
| 66 | 4 | | 1.250988 | 1.161300 | 1.245411 | 1.158231 | 1.250988 | 1.161300 | 1.245411 | 1.158231 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 67 | 5 | | 1.247251 | 1.157641 | 1.241713 | 1.154601 | 1.247251 | 1.157641 | 1.241713 | 1.154601 |
| 68 | 7 | 2 | 1.249451 | 1.194203 | 1.243920 | 1.190150 | 1.244341 | 1.189319 | 1.238833 | 1.185282 |
| 69 | 5 | | 1.247454 | 1.193186 | 1.241934 | 1.189114 | 1.247454 | 1.193186 | 1.241934 | 1.189114 |
| 70 | 6 | 1 | 1.248084 | 1.163371 | 1.242532 | 1.160166 | 1.244924 | 1.160426 | 1.239387 | 1.157229 |
| 71 | 7 | | 1.251368 | 1.188874 | 1.245795 | 1.184987 | 1.251368 | 1.188874 | 1.245795 | 1.184987 |
| 72 | 7 | | 1.247497 | 1.162710 | 1.241948 | 1.159510 | 1.247497 | 1.162710 | 1.241948 | 1.159510 |
| 73 | 5 | | 1.246658 | 1.176782 | 1.241129 | 1.173152 | 1.246658 | 1.176782 | 1.241129 | 1.173152 |
| 74 | 3 | | 1.249203 | 1.183122 | 1.243654 | 1.179363 | 1.249203 | 1.183122 | 1.243654 | 1.179363 |
| 75 | 4 | | 1.249114 | 1.176136 | 1.243577 | 1.172594 | 1.249114 | 1.176136 | 1.243577 | 1.172594 |
| 76 | 9 | 1 | 1.250558 | 1.160351 | 1.244997 | 1.157315 | 1.250057 | 1.159886 | 1.244498 | 1.156851 |
| 77 | 7 | | 1.247133 | 1.160406 | 1.241601 | 1.157282 | 1.247133 | 1.160406 | 1.241601 | 1.157282 |
| 78 | 7 | | 1.247490 | 1.156877 | 1.241958 | 1.153876 | 1.247490 | 1.156877 | 1.241958 | 1.153876 |
| 79 | 9 | | 1.254703 | 1.199084 | 1.249116 | 1.194990 | 1.254703 | 1.199084 | 1.249116 | 1.194990 |
| 80 | 7 | | 1.248943 | 1.155536 | 1.243391 | 1.152607 | 1.248943 | 1.155536 | 1.243391 | 1.152607 |
| 81 | 8 | 1 | 1.250539 | 1.173391 | 1.244981 | 1.169956 | 1.248317 | 1.171306 | 1.242769 | 1.167877 |
| 82 | 6 | 1 | 1.248789 | 1.177284 | 1.243260 | 1.173704 | 1.248735 | 1.177233 | 1.243206 | 1.173654 |
| 83 | 10 | | 1.248971 | 1.178689 | 1.243438 | 1.175071 | 1.248971 | 1.178689 | 1.243438 | 1.175071 |
| 84 | 6 | | 1.250703 | 1.167244 | 1.245132 | 1.163987 | 1.250703 | 1.167244 | 1.245132 | 1.163987 |
| 85 | 6 | | 1.246696 | 1.167894 | 1.241169 | 1.164531 | 1.246696 | 1.167894 | 1.241169 | 1.164531 |
| 86 | 6 | 1 | 1.250971 | 1.160851 | 1.245399 | 1.157800 | 1.249277 | 1.159279 | 1.243712 | 1.156233 |
| 87 | 8 | | 1.249358 | 1.183313 | 1.243820 | 1.179564 | 1.249358 | 1.183313 | 1.243820 | 1.179564 |
| 88 | 7 | | 1.249123 | 1.200640 | 1.243582 | 1.196383 | 1.249123 | 1.200640 | 1.243582 | 1.196383 |
| 89 | 8 | | 1.252853 | 1.179689 | 1.247248 | 1.176088 | 1.252853 | 1.179689 | 1.247248 | 1.176088 |
| 90 | 7 | 1 | 1.249519 | 1.174987 | 1.243972 | 1.171482 | 1.248775 | 1.174287 | 1.243232 | 1.170785 |
| 91 | 8 | | 1.249416 | 1.177152 | 1.243856 | 1.173565 | 1.249416 | 1.177152 | 1.243856 | 1.173565 |
| 92 | 7 | 1 | 1.250559 | 1.188080 | 1.245011 | 1.184219 | 1.250554 | 1.188075 | 1.245005 | 1.184214 |
| 93 | 6 | 2 | 1.249864 | 1.167244 | 1.244280 | 1.163947 | 1.247499 | 1.165036 | 1.241926 | 1.161745 |
| 94 | 7 | | 1.253894 | 1.176946 | 1.248308 | 1.173482 | 1.253894 | 1.176946 | 1.248308 | 1.173482 |
| 95 | 7 | | 1.248857 | 1.159158 | 1.243287 | 1.156090 | 1.248857 | 1.159158 | 1.243287 | 1.156090 |
| 96 | 7 | | 1.252166 | 1.182452 | 1.246606 | 1.178795 | 1.252166 | 1.182452 | 1.246606 | 1.178795 |
| 97 | 9 | 4 | 1.250733 | 1.179159 | 1.245161 | 1.175543 | 1.237777 | 1.166945 | 1.232264 | 1.163366 |
| 98 | 7 | 1 | 1.248732 | 1.191644 | 1.243186 | 1.187626 | 1.237810 | 1.181221 | 1.232312 | 1.177238 |
| 99 | 5 | 1 | 1.248301 | 1.182554 | 1.242760 | 1.178792 | 1.233814 | 1.168830 | 1.228337 | 1.165111 |
| 100 | 7 | | 1.247979 | 1.167933 | 1.242446 | 1.164606 | 1.247979 | 1.167933 | 1.242446 | 1.164606 |

## lg-$^{37}$Cl/$^{35}$Cl isotopic partition-function ratios for [NC···Et···Cl]$^{-}$.*n*DMSO transition structures

| structure sequence number | *n* | number extra imaginaries | extra imaginaries treated as reals | | | | extra imaginaries omitted | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | 300 K | | 303.15K | | 300 K | | 303.15K | |
| | | | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ |
| 1 | 8 | 2 | 1.003197 | 1.002305 | 1.002242 | 1.002220 | 1.001004 | 1.000114 | 1.000919 | 1.000050 |
| 2 | 8 | | 1.003243 | 1.002342 | 1.002279 | 1.002257 | 1.003243 | 1.002342 | 1.003159 | 1.002279 |
| 3 | 4 | 1 | 1.003179 | 1.002362 | 1.002299 | 1.002279 | 1.002701 | 1.001885 | 1.002617 | 1.001821 |
| 4 | 5 | 1 | 1.003112 | 1.002191 | 1.002129 | 1.002107 | 1.003057 | 1.002136 | 1.002973 | 1.002074 |
| 5 | 4 | | 1.003205 | 1.002345 | 1.002282 | 1.002261 | 1.003205 | 1.002345 | 1.003121 | 1.002282 |
| 6 | 4 | 1 | 1.003052 | 1.002179 | 1.002121 | 1.002100 | 1.002255 | 1.001383 | 1.002176 | 1.001325 |
| 7 | 4 | | 1.003273 | 1.002362 | 1.002300 | 1.002278 | 1.003273 | 1.002362 | 1.003188 | 1.002300 |
| 8 | 5 | | 1.003166 | 1.002287 | 1.002225 | 1.002204 | 1.003166 | 1.002287 | 1.003083 | 1.002225 |
| 9 | 3 | | 1.003231 | 1.002397 | 1.002336 | 1.002315 | 1.003231 | 1.002397 | 1.003149 | 1.002336 |
| 10 | 4 | | 1.002863 | 1.001987 | 1.001933 | 1.001912 | 1.002863 | 1.001987 | 1.002787 | 1.001933 |
| 11 | 7 | | 1.002825 | 1.001858 | 1.001805 | 1.001781 | 1.002825 | 1.001858 | 1.002749 | 1.001805 |
| 12 | 8 | | 1.002996 | 1.002044 | 1.001985 | 1.001962 | 1.002996 | 1.002044 | 1.002914 | 1.001985 |
| 13 | 8 | | 1.002597 | 1.001510 | 1.001453 | 1.001428 | 1.002597 | 1.001510 | 1.002515 | 1.001453 |
| 14 | 8 | 1 | 1.003019 | 1.002095 | 1.002036 | 1.002014 | 1.002501 | 1.001578 | 1.002420 | 1.001519 |
| 15 | 6 | | 1.003101 | 1.002214 | 1.002156 | 1.002135 | 1.003101 | 1.002214 | 1.003021 | 1.002156 |
| 16 | 6 | | 1.003183 | 1.002216 | 1.002146 | 1.002123 | 1.003183 | 1.002216 | 1.003090 | 1.002146 |
| 17 | 5 | 1 | 1.003343 | 1.002401 | 1.002335 | 1.002313 | 1.003337 | 1.002394 | 1.003249 | 1.002329 |
| 18 | 5 | | 1.002959 | 1.001783 | 1.001736 | 1.001705 | 1.002959 | 1.001783 | 1.002881 | 1.001736 |
| 19 | 5 | 1 | 1.003167 | 1.002251 | 1.002191 | 1.002169 | 1.001602 | 1.000687 | 1.001520 | 1.000627 |
| 20 | 6 | | 1.003385 | 1.002512 | 1.002452 | 1.002430 | 1.003385 | 1.002512 | 1.003303 | 1.002452 |
| 21 | 6 | | 1.002880 | 1.001662 | 1.001625 | 1.001591 | 1.002880 | 1.001662 | 1.002808 | 1.001625 |
| 22 | 8 | | 1.002666 | 1.001414 | 1.001377 | 1.001344 | 1.002666 | 1.001414 | 1.002596 | 1.001377 |
| 23 | 5 | | 1.002941 | 1.001390 | 1.001344 | 1.001304 | 1.002941 | 1.001390 | 1.002856 | 1.001344 |
| 24 | 7 | 1 | 1.003420 | 1.002502 | 1.002430 | 1.002409 | 1.003407 | 1.002489 | 1.003314 | 1.002417 |
| 25 | 3 | | 1.002156 | 1.001037 | 1.000978 | 1.000952 | 1.002156 | 1.001037 | 1.002071 | 1.000978 |
| 26 | 8 | | 1.002589 | 1.001550 | 1.001496 | 1.001472 | 1.002589 | 1.001550 | 1.002511 | 1.001496 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 27 | 7 | | 1.002786 | 1.001583 | 1.001519 | 1.001491 | 1.002786 | 1.001583 | 1.002693 | 1.001519 |
| 28 | 5 | 1 | 1.002921 | 1.001927 | 1.001876 | 1.001851 | 0.997157 | 0.996169 | 0.997081 | 0.996118 |
| 29 | 6 | | 1.003453 | 1.002653 | 1.002587 | 1.002568 | 1.003453 | 1.002653 | 1.003368 | 1.002587 |
| 30 | 7 | | 1.002755 | 1.001548 | 1.001510 | 1.001478 | 1.002755 | 1.001548 | 1.002684 | 1.001510 |
| 31 | 4 | | 1.003006 | 1.002101 | 1.002034 | 1.002013 | 1.003006 | 1.002101 | 1.002918 | 1.002034 |
| 32 | 5 | | 1.002941 | 1.002026 | 1.001961 | 1.001940 | 1.002941 | 1.002026 | 1.002855 | 1.001961 |
| 33 | 5 | 1 | 1.002519 | 1.001325 | 1.001290 | 1.001258 | 0.987442 | 0.986267 | 0.987376 | 0.986232 |
| 34 | 7 | 1 | 1.003058 | 1.002133 | 1.002071 | 1.002049 | 0.993611 | 0.992694 | 0.993527 | 0.992633 |
| 35 | 3 | | 1.001963 | 1.000830 | 1.000764 | 1.000739 | 1.001963 | 1.000830 | 1.001872 | 1.000764 |
| 36 | 5 | | 1.002907 | 1.001574 | 1.001533 | 1.001497 | 1.002907 | 1.001574 | 1.002830 | 1.001533 |
| 37 | 5 | 1 | 1.003019 | 1.002150 | 1.002085 | 1.002065 | 1.001974 | 1.001106 | 1.001888 | 1.001041 |
| 38 | 7 | 1 | 1.003057 | 1.002132 | 1.002067 | 1.002045 | 1.003002 | 1.002077 | 1.002915 | 1.002011 |
| 39 | 9 | | 1.002995 | 1.001946 | 1.001879 | 1.001855 | 1.002995 | 1.001946 | 1.002904 | 1.001879 |
| 40 | 8 | 1 | 1.002809 | 1.001709 | 1.001651 | 1.001625 | 0.993104 | 0.992016 | 0.993021 | 0.991958 |
| 41 | 6 | 2 | 1.002962 | 1.002088 | 1.002021 | 1.002001 | 0.993858 | 0.992992 | 0.993772 | 0.992926 |
| 42 | 5 | | 1.002904 | 1.002012 | 1.001952 | 1.001931 | 1.002904 | 1.002012 | 1.002823 | 1.001952 |
| 43 | 7 | | 1.003041 | 1.002163 | 1.002105 | 1.002084 | 1.003041 | 1.002163 | 1.002962 | 1.002105 |
| 44 | 7 | | 1.002859 | 1.001904 | 1.001845 | 1.001822 | 1.002859 | 1.001904 | 1.002777 | 1.001845 |
| 45 | 4 | | 1.003172 | 1.002287 | 1.002223 | 1.002202 | 1.003172 | 1.002287 | 1.003087 | 1.002223 |
| 46 | 4 | | 1.002931 | 1.001949 | 1.001890 | 1.001867 | 1.002931 | 1.001949 | 1.002849 | 1.001890 |
| 47 | 6 | 2 | 1.003197 | 1.002363 | 1.002300 | 1.002280 | 1.001134 | 1.000301 | 1.001051 | 1.000238 |
| 48 | 6 | | 1.002975 | 1.002028 | 1.001963 | 1.001941 | 1.002975 | 1.002028 | 1.002888 | 1.001963 |
| 49 | 6 | | 1.003216 | 1.002449 | 1.002376 | 1.002359 | 1.003216 | 1.002449 | 1.003126 | 1.002376 |
| 50 | 7 | | 1.002862 | 1.001987 | 1.001926 | 1.001906 | 1.002862 | 1.001987 | 1.002780 | 1.001926 |
| 51 | 6 | | 1.003032 | 1.001908 | 1.001841 | 1.001815 | 1.003032 | 1.001908 | 1.002939 | 1.001841 |
| 52 | 6 | | 1.002676 | 1.001679 | 1.001630 | 1.001605 | 1.002676 | 1.001679 | 1.002602 | 1.001630 |
| 53 | 4 | | 1.003079 | 1.002206 | 1.002144 | 1.002123 | 1.003079 | 1.002206 | 1.002995 | 1.002144 |
| 54 | 6 | 1 | 1.003159 | 1.002280 | 1.002222 | 1.002200 | 0.989327 | 0.988460 | 0.989248 | 0.988402 |
| 55 | 6 | | 1.003199 | 1.002282 | 1.002217 | 1.002195 | 1.003199 | 1.002282 | 1.003113 | 1.002217 |
| 56 | 6 | | 1.003339 | 1.002449 | 1.002383 | 1.002362 | 1.003339 | 1.002449 | 1.003252 | 1.002383 |
| 57 | 7 | | 1.003230 | 1.002295 | 1.002232 | 1.002209 | 1.003230 | 1.002295 | 1.003145 | 1.002232 |
| 58 | 4 | | 1.003428 | 1.002550 | 1.002488 | 1.002466 | 1.003428 | 1.002550 | 1.003343 | 1.002488 |
| 59 | 6 | | 1.003128 | 1.002257 | 1.002197 | 1.002176 | 1.003128 | 1.002257 | 1.003047 | 1.002197 |
| 60 | 7 | | 1.002786 | 1.001674 | 1.001607 | 1.001582 | 1.002786 | 1.001674 | 1.002694 | 1.001607 |
| 61 | 5 | | 1.003216 | 1.002361 | 1.002300 | 1.002279 | 1.003216 | 1.002361 | 1.003134 | 1.002300 |
| 62 | 6 | 1 | 1.003065 | 1.002125 | 1.002068 | 1.002045 | 1.002161 | 1.001222 | 1.002081 | 1.001166 |
| 63 | 6 | | 1.002763 | 1.001281 | 1.001241 | 1.001202 | 1.002763 | 1.001281 | 1.002684 | 1.001241 |
| 64 | 7 | | 1.002861 | 1.001605 | 1.001564 | 1.001530 | 1.002861 | 1.001605 | 1.002787 | 1.001564 |
| 65 | 6 | | 1.003364 | 1.002543 | 1.002475 | 1.002456 | 1.003364 | 1.002543 | 1.003276 | 1.002475 |
| 66 | 4 | | 1.003425 | 1.002583 | 1.002520 | 1.002499 | 1.003425 | 1.002583 | 1.003341 | 1.002520 |

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|---|---|---|---|---|---|---|---|---|---|---|
| 67 | 5 | | 1.003245 | 1.002343 | 1.002283 | 1.002261 | 1.003245 | 1.002343 | 1.003163 | 1.002283 |
| 68 | 7 | 2 | 1.002786 | 1.001749 | 1.001682 | 1.001658 | 1.002288 | 1.001252 | 1.002197 | 1.001185 |
| 69 | 5 | | 1.003441 | 1.002629 | 1.002551 | 1.002533 | 1.003441 | 1.002629 | 1.003344 | 1.002551 |
| 70 | 6 | 1 | 1.002919 | 1.001971 | 1.001916 | 1.001893 | 1.000751 | 0.999806 | 1.000673 | 0.999750 |
| 71 | 7 | | 1.003129 | 1.002288 | 1.002221 | 1.002201 | 1.003129 | 1.002288 | 1.003042 | 1.002221 |
| 72 | 7 | | 1.003210 | 1.002342 | 1.002280 | 1.002259 | 1.003210 | 1.002342 | 1.003127 | 1.002280 |
| 73 | 5 | | 1.003374 | 1.002597 | 1.002528 | 1.002510 | 1.003374 | 1.002597 | 1.003287 | 1.002528 |
| 74 | 3 | | 1.002745 | 1.001792 | 1.001733 | 1.001711 | 1.002745 | 1.001792 | 1.002663 | 1.001733 |
| 75 | 4 | | 1.003376 | 1.002489 | 1.002421 | 1.002400 | 1.003376 | 1.002489 | 1.003286 | 1.002421 |
| 76 | 9 | 1 | 1.003150 | 1.002213 | 1.002155 | 1.002132 | 1.002551 | 1.001615 | 1.002470 | 1.001557 |
| 77 | 7 | | 1.003023 | 1.002114 | 1.002057 | 1.002035 | 1.003023 | 1.002114 | 1.002944 | 1.002057 |
| 78 | 7 | | 1.003033 | 1.002113 | 1.002058 | 1.002035 | 1.003033 | 1.002113 | 1.002955 | 1.002058 |
| 79 | 9 | | 1.003080 | 1.001958 | 1.001885 | 1.001859 | 1.003080 | 1.001958 | 1.002981 | 1.001885 |
| 80 | 7 | | 1.003397 | 1.002535 | 1.002473 | 1.002451 | 1.003397 | 1.002535 | 1.003313 | 1.002473 |
| 81 | 8 | 1 | 1.002868 | 1.001912 | 1.001856 | 1.001833 | 0.996787 | 0.995837 | 0.996708 | 0.995780 |
| 82 | 6 | 1 | 1.002749 | 1.001807 | 1.001750 | 1.001728 | 1.002743 | 1.001802 | 1.002664 | 1.001745 |
| 83 | 10 | | 1.002794 | 1.001790 | 1.001732 | 1.001708 | 1.002794 | 1.001790 | 1.002712 | 1.001732 |
| 84 | 6 | | 1.003101 | 1.002164 | 1.002105 | 1.002082 | 1.003101 | 1.002164 | 1.003018 | 1.002105 |
| 85 | 6 | | 1.002865 | 1.001908 | 1.001852 | 1.001829 | 1.002865 | 1.001908 | 1.002785 | 1.001852 |
| 86 | 6 | 1 | 1.003039 | 1.002101 | 1.002046 | 1.002022 | 1.000712 | 0.999777 | 1.000633 | 0.999721 |
| 87 | 8 | | 1.002643 | 1.001623 | 1.001566 | 1.001542 | 1.002643 | 1.001623 | 1.002561 | 1.001566 |
| 88 | 7 | | 1.003108 | 1.002345 | 1.002270 | 1.002253 | 1.003108 | 1.002345 | 1.003016 | 1.002270 |
| 89 | 8 | | 1.002954 | 1.002017 | 1.001957 | 1.001935 | 1.002954 | 1.002017 | 1.002872 | 1.001957 |
| 90 | 7 | 1 | 1.002852 | 1.001876 | 1.001818 | 1.001795 | 1.002700 | 1.001725 | 1.002620 | 1.001667 |
| 91 | 8 | | 1.002858 | 1.001904 | 1.001846 | 1.001823 | 1.002858 | 1.001904 | 1.002776 | 1.001846 |
| 92 | 7 | 1 | 1.002868 | 1.001697 | 1.001631 | 1.001604 | 1.002867 | 1.001696 | 1.002774 | 1.001630 |
| 93 | 6 | 2 | 1.003056 | 1.002129 | 1.002070 | 1.002048 | 1.000971 | 1.000046 | 1.000890 | 0.999987 |
| 94 | 7 | | 1.003647 | 1.002704 | 1.002632 | 1.002610 | 1.003647 | 1.002704 | 1.003553 | 1.002632 |
| 95 | 7 | | 1.003081 | 1.002161 | 1.002103 | 1.002081 | 1.003081 | 1.002161 | 1.003001 | 1.002103 |
| 96 | 7 | | 1.002913 | 1.001941 | 1.001880 | 1.001857 | 1.002913 | 1.001941 | 1.002830 | 1.001880 |
| 97 | 9 | 4 | 1.003164 | 1.002288 | 1.002224 | 1.002203 | 0.983896 | 0.983037 | 0.983813 | 0.982974 |
| 98 | 7 | 1 | 1.002981 | 1.002166 | 1.002099 | 1.002080 | 0.999177 | 0.998366 | 0.999092 | 0.998299 |
| 99 | 5 | 1 | 1.003123 | 1.002232 | 1.002165 | 1.002145 | 0.990506 | 0.989626 | 0.990420 | 0.989561 |
| 100 | 7 | | 1.003235 | 1.002253 | 1.002190 | 1.002166 | 1.003235 | 1.002253 | 1.003148 | 1.002190 |

## nu-$^{13}C/^{12}C$ isotopic partition-function ratios for $[NC\cdots Et\cdots Cl]^{-}$.*n*DMSO transition structures

| structure sequence number | *n* | number extra imaginaries | extra imaginaries treated as reals | | | | extra imaginaries omitted | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | 300 K | | 303.15K | | 300 K | | 303.15K | |
| | | | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ |
| 1 | 8 | 2 | 1.118786 | 1.116306 | 1.117074 | 1.114658 | 1.111847 | 1.109383 | 1.110146 | 1.107744 |
| 2 | 8 | | 1.119737 | 1.117451 | 1.118014 | 1.115787 | 1.119737 | 1.117451 | 1.118014 | 1.115787 |
| 3 | 4 | 1 | 1.120021 | 1.117794 | 1.118289 | 1.116120 | 1.120011 | 1.117794 | 1.118280 | 1.116110 |
| 4 | 5 | 1 | 1.118931 | 1.116439 | 1.117215 | 1.114787 | 1.118592 | 1.116439 | 1.116876 | 1.114448 |
| 5 | 4 | | 1.118627 | 1.116256 | 1.116920 | 1.114610 | 1.118627 | 1.116256 | 1.116920 | 1.114610 |
| 6 | 4 | 1 | 1.120214 | 1.117500 | 1.118471 | 1.115827 | 1.119830 | 1.117500 | 1.118088 | 1.115444 |
| 7 | 4 | | 1.119722 | 1.117029 | 1.117993 | 1.115368 | 1.119722 | 1.117029 | 1.117993 | 1.115368 |
| 8 | 5 | | 1.119378 | 1.116737 | 1.117654 | 1.115081 | 1.119378 | 1.116737 | 1.117654 | 1.115081 |
| 9 | 3 | | 1.120119 | 1.117659 | 1.118388 | 1.115991 | 1.120119 | 1.117659 | 1.118388 | 1.115991 |
| 10 | 4 | | 1.119806 | 1.117209 | 1.118078 | 1.115548 | 1.119806 | 1.117209 | 1.118078 | 1.115548 |
| 11 | 7 | | 1.119479 | 1.116869 | 1.117755 | 1.115213 | 1.119479 | 1.116869 | 1.117755 | 1.115213 |
| 12 | 8 | | 1.119664 | 1.117201 | 1.117935 | 1.115535 | 1.119664 | 1.117201 | 1.117935 | 1.115535 |
| 13 | 8 | | 1.118349 | 1.115886 | 1.116639 | 1.114237 | 1.118349 | 1.115886 | 1.116639 | 1.114237 |
| 14 | 8 | 1 | 1.120258 | 1.117882 | 1.118521 | 1.116205 | 1.120151 | 1.117882 | 1.118414 | 1.116098 |
| 15 | 6 | | 1.119124 | 1.116458 | 1.117407 | 1.114810 | 1.119124 | 1.116458 | 1.117407 | 1.114810 |
| 16 | 6 | | 1.118444 | 1.116660 | 1.116748 | 1.115008 | 1.118444 | 1.116660 | 1.116748 | 1.115008 |
| 17 | 5 | 1 | 1.119162 | 1.116601 | 1.117443 | 1.114947 | 1.119155 | 1.116601 | 1.117435 | 1.114940 |
| 18 | 5 | | 1.116048 | 1.108274 | 1.114301 | 1.106738 | 1.116048 | 1.108274 | 1.114301 | 1.106738 |
| 19 | 5 | 1 | 1.119136 | 1.116505 | 1.117419 | 1.114855 | 1.116667 | 1.116505 | 1.114953 | 1.112395 |
| 20 | 6 | | 1.119762 | 1.116699 | 1.118032 | 1.115049 | 1.119762 | 1.116699 | 1.118032 | 1.115049 |
| 21 | 6 | | 1.116075 | 1.104397 | 1.114306 | 1.102969 | 1.116075 | 1.104397 | 1.114306 | 1.102969 |
| 22 | 8 | | 1.114274 | 1.102303 | 1.112515 | 1.100883 | 1.114274 | 1.102303 | 1.112515 | 1.100883 |
| 23 | 5 | | 1.111467 | 1.100773 | 1.109752 | 1.099346 | 1.111467 | 1.100773 | 1.109752 | 1.099346 |
| 24 | 7 | 1 | 1.118497 | 1.116667 | 1.116803 | 1.115019 | 1.118492 | 1.116667 | 1.116799 | 1.115015 |
| 25 | 3 | | 1.117907 | 1.116003 | 1.116204 | 1.114347 | 1.117907 | 1.116003 | 1.116204 | 1.114347 |
| 26 | 8 | | 1.120106 | 1.117960 | 1.118371 | 1.116279 | 1.120106 | 1.117960 | 1.118371 | 1.116279 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 27 | 7 | | 1.118564 | 1.116762 | 1.116865 | 1.115107 | 1.118564 | 1.116762 | 1.116865 | 1.115107 |
| 28 | 5 | 1 | 1.119388 | 1.115883 | 1.117652 | 1.114240 | 1.118723 | 1.115883 | 1.116988 | 1.113577 |
| 29 | 6 | | 1.119643 | 1.116794 | 1.117913 | 1.115138 | 1.119643 | 1.116794 | 1.117913 | 1.115138 |
| 30 | 7 | | 1.113608 | 1.100702 | 1.111851 | 1.099312 | 1.113608 | 1.100702 | 1.111851 | 1.099312 |
| 31 | 4 | | 1.118787 | 1.116973 | 1.117081 | 1.115313 | 1.118787 | 1.116973 | 1.117081 | 1.115313 |
| 32 | 5 | | 1.119566 | 1.117862 | 1.117849 | 1.116187 | 1.119566 | 1.117862 | 1.117849 | 1.116187 |
| 33 | 5 | 1 | 1.115838 | 1.105817 | 1.114073 | 1.104333 | 1.115378 | 1.105817 | 1.113614 | 1.103878 |
| 34 | 7 | 1 | 1.119602 | 1.117398 | 1.117878 | 1.115730 | 1.119546 | 1.117398 | 1.117823 | 1.115674 |
| 35 | 3 | | 1.116219 | 1.114917 | 1.114563 | 1.113291 | 1.116219 | 1.114917 | 1.114563 | 1.113291 |
| 36 | 5 | | 1.114159 | 1.101251 | 1.112387 | 1.099843 | 1.114159 | 1.101251 | 1.112387 | 1.099843 |
| 37 | 5 | 1 | 1.119909 | 1.117797 | 1.118172 | 1.116112 | 1.119905 | 1.117797 | 1.118168 | 1.116108 |
| 38 | 7 | 1 | 1.118905 | 1.117129 | 1.117204 | 1.115472 | 1.118845 | 1.117129 | 1.117145 | 1.115413 |
| 39 | 9 | | 1.118757 | 1.117040 | 1.117058 | 1.115384 | 1.118757 | 1.117040 | 1.117058 | 1.115384 |
| 40 | 8 | 1 | 1.119153 | 1.117003 | 1.117440 | 1.115344 | 1.117653 | 1.117003 | 1.115942 | 1.113849 |
| 41 | 6 | 2 | 1.118541 | 1.117007 | 1.116848 | 1.115352 | 1.113266 | 1.117007 | 1.111580 | 1.110092 |
| 42 | 5 | | 1.119411 | 1.117461 | 1.117695 | 1.115794 | 1.119411 | 1.117461 | 1.117695 | 1.115794 |
| 43 | 7 | | 1.119121 | 1.116693 | 1.117410 | 1.115045 | 1.119121 | 1.116693 | 1.117410 | 1.115045 |
| 44 | 7 | | 1.119209 | 1.116948 | 1.117488 | 1.115284 | 1.119209 | 1.116948 | 1.117488 | 1.115284 |
| 45 | 4 | | 1.119627 | 1.117525 | 1.117906 | 1.115858 | 1.119627 | 1.117525 | 1.117906 | 1.115858 |
| 46 | 4 | | 1.119756 | 1.117385 | 1.118025 | 1.115714 | 1.119756 | 1.117385 | 1.118025 | 1.115714 |
| 47 | 6 | 2 | 1.118951 | 1.116458 | 1.117234 | 1.114805 | 1.118844 | 1.116458 | 1.117128 | 1.114698 |
| 48 | 6 | | 1.119246 | 1.117432 | 1.117534 | 1.115764 | 1.119246 | 1.117432 | 1.117534 | 1.115764 |
| 49 | 6 | | 1.118252 | 1.116797 | 1.116565 | 1.115146 | 1.118252 | 1.116797 | 1.116565 | 1.115146 |
| 50 | 7 | | 1.118692 | 1.116789 | 1.116990 | 1.115135 | 1.118692 | 1.116789 | 1.116990 | 1.115135 |
| 51 | 6 | | 1.118497 | 1.116552 | 1.116796 | 1.114899 | 1.118497 | 1.116552 | 1.116796 | 1.114899 |
| 52 | 6 | | 1.119923 | 1.117065 | 1.118183 | 1.115400 | 1.119923 | 1.117065 | 1.118183 | 1.115400 |
| 53 | 4 | | 1.119828 | 1.117621 | 1.118099 | 1.115947 | 1.119828 | 1.117621 | 1.118099 | 1.115947 |
| 54 | 6 | 1 | 1.120257 | 1.117521 | 1.118518 | 1.115853 | 1.120105 | 1.117521 | 1.118366 | 1.115701 |
| 55 | 6 | | 1.118369 | 1.115963 | 1.116665 | 1.114321 | 1.118369 | 1.115963 | 1.116665 | 1.114321 |
| 56 | 6 | | 1.118580 | 1.116334 | 1.116877 | 1.114689 | 1.118580 | 1.116334 | 1.116877 | 1.114689 |
| 57 | 7 | | 1.119458 | 1.117091 | 1.117737 | 1.115430 | 1.119458 | 1.117091 | 1.117737 | 1.115430 |
| 58 | 4 | | 1.119282 | 1.115832 | 1.117548 | 1.114188 | 1.119282 | 1.115832 | 1.117548 | 1.114188 |
| 59 | 6 | | 1.119967 | 1.117620 | 1.118238 | 1.115952 | 1.119967 | 1.117620 | 1.118238 | 1.115952 |
| 60 | 7 | | 1.117642 | 1.116084 | 1.115966 | 1.114446 | 1.117642 | 1.116084 | 1.115966 | 1.114446 |
| 61 | 5 | | 1.119497 | 1.116993 | 1.117774 | 1.115334 | 1.119497 | 1.116993 | 1.117774 | 1.115334 |
| 62 | 6 | 1 | 1.119941 | 1.117140 | 1.118204 | 1.115476 | 1.119442 | 1.117140 | 1.117706 | 1.114979 |
| 63 | 6 | | 1.117741 | 1.110953 | 1.115980 | 1.109378 | 1.117741 | 1.110953 | 1.115980 | 1.109378 |
| 64 | 7 | | 1.113528 | 1.101310 | 1.111774 | 1.099899 | 1.113528 | 1.101310 | 1.111774 | 1.099899 |
| 65 | 6 | | 1.119859 | 1.117880 | 1.118134 | 1.116205 | 1.119859 | 1.117880 | 1.118134 | 1.116205 |
| 66 | 4 | | 1.118943 | 1.115557 | 1.117217 | 1.113919 | 1.118943 | 1.115557 | 1.117217 | 1.113919 |

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|---|---|---|---|---|---|---|---|---|---|---|
| 67 | 5 | | 1.119751 | 1.116853 | 1.118019 | 1.115196 | 1.119751 | 1.116853 | 1.118019 | 1.115196 |
| 68 | 7 | 2 | 1.118508 | 1.117035 | 1.116815 | 1.115379 | 1.116308 | 1.117035 | 1.114619 | 1.113185 |
| 69 | 5 | | 1.118811 | 1.117342 | 1.117110 | 1.115678 | 1.118811 | 1.117342 | 1.117110 | 1.115678 |
| 70 | 6 | 1 | 1.119918 | 1.117512 | 1.118189 | 1.115845 | 1.119611 | 1.117512 | 1.117882 | 1.115539 |
| 71 | 7 | | 1.118216 | 1.116461 | 1.116527 | 1.114816 | 1.118216 | 1.116461 | 1.116527 | 1.114816 |
| 72 | 7 | | 1.119903 | 1.117418 | 1.118174 | 1.115753 | 1.119903 | 1.117418 | 1.118174 | 1.115753 |
| 73 | 5 | | 1.118739 | 1.116689 | 1.117037 | 1.115039 | 1.118739 | 1.116689 | 1.117037 | 1.115039 |
| 74 | 3 | | 1.119353 | 1.117570 | 1.117640 | 1.115901 | 1.119353 | 1.117570 | 1.117640 | 1.115901 |
| 75 | 4 | | 1.119459 | 1.117177 | 1.117735 | 1.115510 | 1.119459 | 1.117177 | 1.117735 | 1.115510 |
| 76 | 9 | 1 | 1.119955 | 1.116858 | 1.118213 | 1.115197 | 1.119815 | 1.116858 | 1.118074 | 1.115058 |
| 77 | 7 | | 1.120538 | 1.117941 | 1.118793 | 1.116262 | 1.120538 | 1.117941 | 1.118793 | 1.116262 |
| 78 | 7 | | 1.120013 | 1.117222 | 1.118275 | 1.115557 | 1.120013 | 1.117222 | 1.118275 | 1.115557 |
| 79 | 9 | | 1.117653 | 1.115987 | 1.115972 | 1.114346 | 1.117653 | 1.115987 | 1.115972 | 1.114346 |
| 80 | 7 | | 1.119718 | 1.116579 | 1.117983 | 1.114927 | 1.119718 | 1.116579 | 1.117983 | 1.114927 |
| 81 | 8 | 1 | 1.119143 | 1.116716 | 1.117425 | 1.115060 | 1.118938 | 1.116716 | 1.117221 | 1.114856 |
| 82 | 6 | 1 | 1.119110 | 1.116959 | 1.117393 | 1.115296 | 1.119042 | 1.116959 | 1.117325 | 1.115229 |
| 83 | 10 | | 1.119247 | 1.117015 | 1.117526 | 1.115350 | 1.119247 | 1.117015 | 1.117526 | 1.115350 |
| 84 | 6 | | 1.119268 | 1.116575 | 1.117546 | 1.114923 | 1.119268 | 1.116575 | 1.117546 | 1.114923 |
| 85 | 6 | | 1.120209 | 1.118068 | 1.118476 | 1.116390 | 1.120209 | 1.118068 | 1.118476 | 1.116390 |
| 86 | 6 | 1 | 1.119023 | 1.116051 | 1.117304 | 1.114410 | 1.118939 | 1.116051 | 1.117219 | 1.114326 |
| 87 | 8 | | 1.118648 | 1.116727 | 1.116946 | 1.115073 | 1.118648 | 1.116727 | 1.116946 | 1.115073 |
| 88 | 7 | | 1.118108 | 1.116862 | 1.116425 | 1.115209 | 1.118108 | 1.116862 | 1.116425 | 1.115209 |
| 89 | 8 | | 1.118716 | 1.116488 | 1.117011 | 1.114839 | 1.118716 | 1.116488 | 1.117011 | 1.114839 |
| 90 | 7 | 1 | 1.119143 | 1.116761 | 1.117425 | 1.115103 | 1.118170 | 1.116761 | 1.116454 | 1.114134 |
| 91 | 8 | | 1.119123 | 1.117130 | 1.117414 | 1.115471 | 1.119123 | 1.117130 | 1.117414 | 1.115471 |
| 92 | 7 | 1 | 1.118465 | 1.116827 | 1.116774 | 1.115176 | 1.118462 | 1.116827 | 1.116771 | 1.115173 |
| 93 | 6 | 2 | 1.119943 | 1.117361 | 1.118208 | 1.115692 | 1.119599 | 1.117361 | 1.117864 | 1.115349 |
| 94 | 7 | | 1.118328 | 1.115640 | 1.116621 | 1.114001 | 1.118328 | 1.115640 | 1.116621 | 1.114001 |
| 95 | 7 | | 1.120194 | 1.117548 | 1.118456 | 1.115879 | 1.120194 | 1.117548 | 1.118456 | 1.115879 |
| 96 | 7 | | 1.119208 | 1.116594 | 1.117478 | 1.114930 | 1.119208 | 1.116594 | 1.117478 | 1.114930 |
| 97 | 9 | 4 | 1.119550 | 1.117364 | 1.117826 | 1.115695 | 1.117692 | 1.117364 | 1.115971 | 1.113843 |
| 98 | 7 | 1 | 1.118566 | 1.117035 | 1.116872 | 1.115379 | 1.113940 | 1.117035 | 1.112254 | 1.110767 |
| 99 | 5 | 1 | 1.118942 | 1.117133 | 1.117237 | 1.115474 | 1.117254 | 1.117133 | 1.115552 | 1.113791 |
| 100 | 7 | | 1.119781 | 1.117231 | 1.118049 | 1.115564 | 1.119781 | 1.117231 | 1.118049 | 1.115564 |

## nu-$^{15}$N/$^{14}$N isotopic partition-function ratios for [NC···Et···Cl]$^{-}$.*n*DMSO transition structures

| structure sequence number | *n* | number extra imaginaries | extra imaginaries treated as reals | | | | extra imaginaries omitted | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | 300 K | | 303.15K | | 300 K | | 303.15K | |
| | | | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ | $f_{TS}$ | $(f_{TS})_{corr}$ |
| 1 | 8 | 2 | 1.078337 | 1.076049 | 1.077239 | 1.075007 | 1.070751 | 1.068479 | 1.069661 | 1.067445 |
| 2 | 8 | | 1.079101 | 1.076963 | 1.077993 | 1.075909 | 1.079101 | 1.076963 | 1.077993 | 1.075909 |
| 3 | 4 | 1 | 1.078967 | 1.076990 | 1.077863 | 1.075934 | 1.078961 | 1.076984 | 1.077856 | 1.075928 |
| 4 | 5 | 1 | 1.077990 | 1.075818 | 1.076900 | 1.074782 | 1.077687 | 1.075515 | 1.076597 | 1.074479 |
| 5 | 4 | | 1.077185 | 1.075075 | 1.076113 | 1.074055 | 1.077185 | 1.075075 | 1.076113 | 1.074055 |
| 6 | 4 | 1 | 1.077642 | 1.075215 | 1.076560 | 1.074195 | 1.077235 | 1.074809 | 1.076154 | 1.073790 |
| 7 | 4 | | 1.080012 | 1.077626 | 1.078883 | 1.076557 | 1.080012 | 1.077626 | 1.078883 | 1.076557 |
| 8 | 5 | | 1.079865 | 1.077773 | 1.078744 | 1.076704 | 1.079865 | 1.077773 | 1.078744 | 1.076704 |
| 9 | 3 | | 1.078449 | 1.076185 | 1.077356 | 1.075149 | 1.078449 | 1.076185 | 1.077356 | 1.075149 |
| 10 | 4 | | 1.077979 | 1.075639 | 1.076893 | 1.074613 | 1.077979 | 1.075639 | 1.076893 | 1.074613 |
| 11 | 7 | | 1.077866 | 1.075462 | 1.076780 | 1.074437 | 1.077866 | 1.075462 | 1.076780 | 1.074437 |
| 12 | 8 | | 1.079097 | 1.076915 | 1.077985 | 1.075858 | 1.079097 | 1.076915 | 1.077985 | 1.075858 |
| 13 | 8 | | 1.077737 | 1.075970 | 1.076657 | 1.074934 | 1.077737 | 1.075970 | 1.076657 | 1.074934 |
| 14 | 8 | 1 | 1.078033 | 1.075781 | 1.076942 | 1.074746 | 1.077931 | 1.075679 | 1.076841 | 1.074645 |
| 15 | 6 | | 1.078462 | 1.076029 | 1.077363 | 1.074992 | 1.078462 | 1.076029 | 1.077363 | 1.074992 |
| 16 | 6 | | 1.077848 | 1.076416 | 1.076770 | 1.075373 | 1.077848 | 1.076416 | 1.076770 | 1.075373 |
| 17 | 5 | 1 | 1.077770 | 1.075421 | 1.076682 | 1.074393 | 1.077764 | 1.075416 | 1.076677 | 1.074387 |
| 18 | 5 | | 1.079657 | 1.077501 | 1.078550 | 1.076451 | 1.079657 | 1.077501 | 1.078550 | 1.076451 |
| 19 | 5 | 1 | 1.079015 | 1.076764 | 1.077907 | 1.075712 | 1.076500 | 1.074254 | 1.075395 | 1.073205 |
| 20 | 6 | | 1.079691 | 1.076907 | 1.078572 | 1.075860 | 1.079691 | 1.076907 | 1.078572 | 1.075860 |
| 21 | 6 | | 1.080037 | 1.077556 | 1.078931 | 1.076521 | 1.080037 | 1.077556 | 1.078931 | 1.076521 |
| 22 | 8 | | 1.080075 | 1.078207 | 1.078969 | 1.077154 | 1.080075 | 1.078207 | 1.078969 | 1.077154 |
| 23 | 5 | | 1.080712 | 1.079287 | 1.079595 | 1.078207 | 1.080712 | 1.079287 | 1.079595 | 1.078207 |
| 24 | 7 | 1 | 1.078335 | 1.076582 | 1.077243 | 1.075533 | 1.078331 | 1.076578 | 1.077240 | 1.075530 |
| 25 | 3 | | 1.077609 | 1.076436 | 1.076536 | 1.075392 | 1.077609 | 1.076436 | 1.076536 | 1.075392 |
| 26 | 8 | | 1.078013 | 1.076191 | 1.076929 | 1.075152 | 1.078013 | 1.076191 | 1.076929 | 1.075152 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 27 | 7 | | 1.077835 | 1.076217 | 1.076753 | 1.075174 | 1.077835 | 1.076217 | 1.076753 | 1.075174 |
| 28 | 5 | 1 | 1.078187 | 1.075367 | 1.077092 | 1.074345 | 1.077917 | 1.075099 | 1.076823 | 1.074077 |
| 29 | 6 | | 1.077781 | 1.075388 | 1.076700 | 1.074368 | 1.077781 | 1.075388 | 1.076700 | 1.074368 |
| 30 | 7 | | 1.080691 | 1.078760 | 1.079572 | 1.077695 | 1.080691 | 1.078760 | 1.079572 | 1.077695 |
| 31 | 4 | | 1.077296 | 1.075916 | 1.076230 | 1.074883 | 1.077296 | 1.075916 | 1.076230 | 1.074883 |
| 32 | 5 | | 1.077989 | 1.076519 | 1.076907 | 1.075472 | 1.077989 | 1.076519 | 1.076907 | 1.075472 |
| 33 | 5 | 1 | 1.080017 | 1.077871 | 1.078908 | 1.076821 | 1.079272 | 1.077127 | 1.078164 | 1.076078 |
| 34 | 7 | 1 | 1.077982 | 1.076134 | 1.076898 | 1.075095 | 1.077948 | 1.076099 | 1.076863 | 1.075060 |
| 35 | 3 | | 1.077301 | 1.076143 | 1.076221 | 1.075091 | 1.077301 | 1.076143 | 1.076221 | 1.075091 |
| 36 | 5 | | 1.081054 | 1.079373 | 1.079931 | 1.078297 | 1.081054 | 1.079373 | 1.079931 | 1.078297 |
| 37 | 5 | 1 | 1.078995 | 1.077372 | 1.077888 | 1.076305 | 1.078985 | 1.077363 | 1.077879 | 1.076296 |
| 38 | 7 | 1 | 1.077762 | 1.076142 | 1.076683 | 1.075103 | 1.077650 | 1.076030 | 1.076571 | 1.074990 |
| 39 | 9 | | 1.077620 | 1.076157 | 1.076546 | 1.075118 | 1.077620 | 1.076157 | 1.076546 | 1.075118 |
| 40 | 8 | 1 | 1.077530 | 1.075538 | 1.076451 | 1.074509 | 1.076121 | 1.074132 | 1.075044 | 1.073105 |
| 41 | 6 | 2 | 1.077354 | 1.075878 | 1.076280 | 1.074839 | 1.072006 | 1.070537 | 1.070937 | 1.069503 |
| 42 | 5 | | 1.077787 | 1.075984 | 1.076705 | 1.074947 | 1.077787 | 1.075984 | 1.076705 | 1.074947 |
| 43 | 7 | | 1.077654 | 1.075376 | 1.076574 | 1.074353 | 1.077654 | 1.075376 | 1.076574 | 1.074353 |
| 44 | 7 | | 1.077855 | 1.075755 | 1.076764 | 1.074716 | 1.077855 | 1.075755 | 1.076764 | 1.074716 |
| 45 | 4 | | 1.077831 | 1.075909 | 1.076748 | 1.074874 | 1.077831 | 1.075909 | 1.076748 | 1.074874 |
| 46 | 4 | | 1.077991 | 1.076038 | 1.076907 | 1.075002 | 1.077991 | 1.076038 | 1.076907 | 1.075002 |
| 47 | 6 | 2 | 1.077930 | 1.075743 | 1.076843 | 1.074710 | 1.077743 | 1.075556 | 1.076657 | 1.074524 |
| 48 | 6 | | 1.077648 | 1.076020 | 1.076571 | 1.074982 | 1.077648 | 1.076020 | 1.076571 | 1.074982 |
| 49 | 6 | | 1.077173 | 1.075812 | 1.076103 | 1.074775 | 1.077173 | 1.075812 | 1.076103 | 1.074775 |
| 50 | 7 | | 1.077832 | 1.076009 | 1.076745 | 1.074967 | 1.077832 | 1.076009 | 1.076745 | 1.074967 |
| 51 | 6 | | 1.077754 | 1.076009 | 1.076669 | 1.074966 | 1.077754 | 1.076009 | 1.076669 | 1.074966 |
| 52 | 6 | | 1.078601 | 1.076189 | 1.077502 | 1.075150 | 1.078601 | 1.076189 | 1.077502 | 1.075150 |
| 53 | 4 | | 1.078521 | 1.076682 | 1.077427 | 1.075633 | 1.078521 | 1.076682 | 1.077427 | 1.075633 |
| 54 | 6 | 1 | 1.077845 | 1.075390 | 1.076762 | 1.074371 | 1.077801 | 1.075347 | 1.076719 | 1.074327 |
| 55 | 6 | | 1.077270 | 1.075327 | 1.076199 | 1.074304 | 1.077270 | 1.075327 | 1.076199 | 1.074304 |
| 56 | 6 | | 1.077579 | 1.075405 | 1.076495 | 1.074375 | 1.077579 | 1.075405 | 1.076495 | 1.074375 |
| 57 | 7 | | 1.078203 | 1.076050 | 1.077114 | 1.075015 | 1.078203 | 1.076050 | 1.077114 | 1.075015 |
| 58 | 4 | | 1.079378 | 1.076875 | 1.078266 | 1.075827 | 1.079378 | 1.076875 | 1.078266 | 1.075827 |
| 59 | 6 | | 1.078716 | 1.076609 | 1.077618 | 1.075565 | 1.078716 | 1.076609 | 1.077618 | 1.075565 |
| 60 | 7 | | 1.076800 | 1.075384 | 1.075739 | 1.074357 | 1.076800 | 1.075384 | 1.075739 | 1.074357 |
| 61 | 5 | | 1.078673 | 1.076328 | 1.077569 | 1.075284 | 1.078673 | 1.076328 | 1.077569 | 1.075284 |
| 62 | 6 | 1 | 1.077899 | 1.075302 | 1.076808 | 1.074277 | 1.077594 | 1.074998 | 1.076504 | 1.073973 |
| 63 | 6 | | 1.079758 | 1.077431 | 1.078648 | 1.076383 | 1.079758 | 1.077431 | 1.078648 | 1.076383 |
| 64 | 7 | | 1.080386 | 1.078609 | 1.079275 | 1.077546 | 1.080386 | 1.078609 | 1.079275 | 1.077546 |
| 65 | 6 | | 1.077907 | 1.076084 | 1.076824 | 1.075045 | 1.077907 | 1.076084 | 1.076824 | 1.075045 |
| 66 | 4 | | 1.078290 | 1.075909 | 1.077201 | 1.074881 | 1.078290 | 1.075909 | 1.077201 | 1.074881 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 67 | 5 | | 1.078177 | 1.075911 | 1.077092 | 1.074883 | 1.078177 | 1.075911 | 1.077092 | 1.074883 |
| 68 | 7 | 2 | 1.077405 | 1.076047 | 1.076333 | 1.075007 | 1.075054 | 1.073698 | 1.073984 | 1.072661 |
| 69 | 5 | | 1.077225 | 1.075876 | 1.076155 | 1.074839 | 1.077225 | 1.075876 | 1.076155 | 1.074839 |
| 70 | 6 | 1 | 1.078501 | 1.076305 | 1.077407 | 1.075266 | 1.078289 | 1.076093 | 1.077195 | 1.075054 |
| 71 | 7 | | 1.076876 | 1.075151 | 1.075809 | 1.074126 | 1.076876 | 1.075151 | 1.075809 | 1.074126 |
| 72 | 7 | | 1.078921 | 1.076674 | 1.077818 | 1.075627 | 1.078921 | 1.076674 | 1.077818 | 1.075627 |
| 73 | 5 | | 1.078223 | 1.076468 | 1.077135 | 1.075423 | 1.078223 | 1.076468 | 1.077135 | 1.075423 |
| 74 | 3 | | 1.077908 | 1.076204 | 1.076823 | 1.075161 | 1.077908 | 1.076204 | 1.076823 | 1.075161 |
| 75 | 4 | | 1.078361 | 1.076302 | 1.077261 | 1.075254 | 1.078361 | 1.076302 | 1.077261 | 1.075254 |
| 76 | 9 | 1 | 1.078517 | 1.075749 | 1.077416 | 1.074719 | 1.078344 | 1.075577 | 1.077244 | 1.074547 |
| 77 | 7 | | 1.078009 | 1.075705 | 1.076922 | 1.074677 | 1.078009 | 1.075705 | 1.076922 | 1.074677 |
| 78 | 7 | | 1.079515 | 1.076988 | 1.078394 | 1.075932 | 1.079515 | 1.076988 | 1.078394 | 1.075932 |
| 79 | 9 | | 1.076883 | 1.075459 | 1.075821 | 1.074431 | 1.076883 | 1.075459 | 1.075821 | 1.074431 |
| 80 | 7 | | 1.078797 | 1.076019 | 1.077691 | 1.074984 | 1.078797 | 1.076019 | 1.077691 | 1.074984 |
| 81 | 8 | 1 | 1.077304 | 1.075087 | 1.076229 | 1.074067 | 1.077028 | 1.074811 | 1.075953 | 1.073791 |
| 82 | 6 | 1 | 1.077192 | 1.075190 | 1.076115 | 1.074163 | 1.077072 | 1.075071 | 1.075995 | 1.074043 |
| 83 | 10 | | 1.078213 | 1.076387 | 1.077122 | 1.075341 | 1.078213 | 1.076387 | 1.077122 | 1.075341 |
| 84 | 6 | | 1.077551 | 1.075217 | 1.076473 | 1.074198 | 1.077551 | 1.075217 | 1.076473 | 1.074198 |
| 85 | 6 | | 1.077806 | 1.075759 | 1.076724 | 1.074728 | 1.077806 | 1.075759 | 1.076724 | 1.074728 |
| 86 | 6 | 1 | 1.078056 | 1.075456 | 1.076966 | 1.074432 | 1.078023 | 1.075424 | 1.076933 | 1.074400 |
| 87 | 8 | | 1.077381 | 1.075691 | 1.076308 | 1.074659 | 1.077381 | 1.075691 | 1.076308 | 1.074659 |
| 88 | 7 | | 1.077248 | 1.075999 | 1.076175 | 1.074955 | 1.077248 | 1.075999 | 1.076175 | 1.074955 |
| 89 | 8 | | 1.077639 | 1.075577 | 1.076557 | 1.074546 | 1.077639 | 1.075577 | 1.076557 | 1.074546 |
| 90 | 7 | 1 | 1.077927 | 1.075882 | 1.076839 | 1.074845 | 1.076171 | 1.074130 | 1.075085 | 1.073094 |
| 91 | 8 | | 1.077873 | 1.075975 | 1.076787 | 1.074937 | 1.077873 | 1.075975 | 1.076787 | 1.074937 |
| 92 | 7 | 1 | 1.077720 | 1.076180 | 1.076643 | 1.075140 | 1.077717 | 1.076177 | 1.076640 | 1.075137 |
| 93 | 6 | 2 | 1.078492 | 1.076355 | 1.077395 | 1.075312 | 1.078302 | 1.076166 | 1.077205 | 1.075123 |
| 94 | 7 | | 1.078747 | 1.076266 | 1.077635 | 1.075216 | 1.078747 | 1.076266 | 1.077635 | 1.075216 |
| 95 | 7 | | 1.079006 | 1.076577 | 1.077899 | 1.075532 | 1.079006 | 1.076577 | 1.077899 | 1.075532 |
| 96 | 7 | | 1.078076 | 1.076263 | 1.076990 | 1.075222 | 1.078076 | 1.076263 | 1.076990 | 1.075222 |
| 97 | 9 | 4 | 1.077695 | 1.075719 | 1.076612 | 1.074684 | 1.075030 | 1.073059 | 1.073949 | 1.072026 |
| 98 | 7 | 1 | 1.077758 | 1.076353 | 1.076679 | 1.075307 | 1.072607 | 1.071208 | 1.071533 | 1.070167 |
| 99 | 5 | 1 | 1.077859 | 1.076105 | 1.076771 | 1.075060 | 1.076936 | 1.075184 | 1.075849 | 1.074140 |
| 100 | 7 | | 1.078713 | 1.076642 | 1.077615 | 1.075596 | 1.078713 | 1.076642 | 1.077615 | 1.075596 |

## $\alpha$-$D_2$/$\alpha$-$H_2$ isotopic partition-function ratios for ($NC^{-}\cdots EtCl$).*n*DMSO reactant structures:

| structure sequence number | *n* | number extra imaginaries | extra imaginaries treated as reals: 300 K $f_{RS}$ | extra imaginaries treated as reals: 303.15K $f_{RS}$ | extra imaginaries omitted: 300 K $f_{RS}$ | extra imaginaries omitted: 303.15K $f_{RS}$ |
|---|---|---|---|---|---|---|
| 1 | 4 | | 1.485658 | 1.487392 | 1.496313 | 1.487392 |
| 2 | 5 | 1 | 1.489546 | 1.480933 | 1.466005 | 1.457355 |
| 3 | 4 | | 1.489312 | 1.485943 | 1.494842 | 1.485943 |
| 4 | 4 | | 1.494034 | 1.485614 | 1.494518 | 1.485614 |
| 5 | 4 | | 1.492251 | 1.484102 | 1.492956 | 1.484102 |
| 6 | 7 | | 1.492662 | 1.484928 | 1.493801 | 1.484928 |
| 7 | 3 | | 1.495041 | 1.483348 | 1.492183 | 1.483348 |
| 8 | 6 | 1 | 1.489251 | 1.480280 | 1.489054 | 1.480280 |
| 9 | 5 | | 1.491427 | 1.484418 | 1.493281 | 1.484418 |
| 10 | 1 | 10 | 1.490087 | 1.457695 | 1.389013 | 1.381033 |
| 11 | 4 | 1 | 1.490570 | 1.483660 | 1.492465 | 1.483616 |
| 12 | 3 | | 1.490085 | 1.478033 | 1.486766 | 1.478033 |
| 13 | 4 | | 1.486591 | 1.483775 | 1.492627 | 1.483775 |
| 14 | 5 | | 1.489969 | 1.487842 | 1.496775 | 1.487842 |
| 15 | 5 | | 1.487888 | 1.483187 | 1.492029 | 1.483187 |
| 16 | 4 | 2 | 1.488601 | 1.481520 | 1.453649 | 1.445061 |
| 17 | 7 | 1 | 1.488431 | 1.485199 | 1.493392 | 1.484520 |
| 18 | 5 | | 1.490577 | 1.480582 | 1.489362 | 1.480583 |
| 19 | 3 | | 1.494932 | 1.483431 | 1.492273 | 1.483431 |
| 20 | 2 | | 1.490487 | 1.478435 | 1.487171 | 1.478435 |
| 21 | 3 | | 1.492495 | 1.485187 | 1.494071 | 1.485187 |
| 22 | 5 | | 1.487931 | 1.481461 | 1.490257 | 1.481461 |
| 23 | 2 | | 1.493347 | 1.481878 | 1.490685 | 1.481878 |
| 24 | 4 | | 1.490277 | 1.479312 | 1.488069 | 1.479312 |
| 25 | 3 | | 1.495011 | 1.486655 | 1.495560 | 1.486655 |
| 26 | 5 | | 1.490232 | 1.480524 | 1.489303 | 1.480524 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 27 | 6 | | 1.488479 | 1.479836 | 1.488606 | 1.479836 |
| 28 | 5 | | 1.489360 | 1.480901 | 1.489692 | 1.480901 |
| 29 | 6 | | 1.491543 | 1.485622 | 1.494538 | 1.485623 |
| 30 | 5 | 1 | 1.492838 | 1.484653 | 1.471887 | 1.463152 |
| 31 | 4 | | 1.487960 | 1.487058 | 1.495970 | 1.487058 |
| 32 | 3 | | 1.481694 | 1.482000 | 1.490813 | 1.482000 |
| 33 | 2 | | 1.490343 | 1.483105 | 1.491939 | 1.483105 |
| 34 | 5 | | 1.492925 | 1.480974 | 1.489765 | 1.480974 |
| 35 | 6 | | 1.490406 | 1.484410 | 1.493281 | 1.484410 |
| 36 | 6 | | 1.491229 | 1.484540 | 1.493418 | 1.484541 |
| 37 | 5 | | 1.493200 | 1.484620 | 1.493492 | 1.484620 |
| 38 | 5 | | 1.490195 | 1.480829 | 1.489625 | 1.480829 |
| 39 | 4 | | 1.491176 | 1.482250 | 1.491064 | 1.482250 |
| 40 | 5 | 1 | 1.488048 | 1.482946 | 1.489022 | 1.480194 |
| 41 | 5 | | 1.488002 | 1.481975 | 1.490785 | 1.481975 |
| 42 | 4 | | 1.489745 | 1.478909 | 1.487659 | 1.478909 |
| 43 | 2 | | 1.487639 | 1.482276 | 1.491096 | 1.482276 |
| 44 | 6 | | 1.490662 | 1.484164 | 1.493029 | 1.484164 |
| 45 | 5 | 1 | 1.490754 | 1.480592 | 1.485975 | 1.477208 |
| 46 | 4 | | 1.489568 | 1.484434 | 1.493292 | 1.484434 |
| 47 | 4 | 1 | 1.490479 | 1.484164 | 1.492985 | 1.484124 |
| 48 | 3 | | 1.491059 | 1.484271 | 1.493128 | 1.484271 |
| 49 | 4 | | 1.492961 | 1.483226 | 1.492060 | 1.483226 |
| 50 | 4 | | 1.488396 | 1.483608 | 1.492458 | 1.483608 |
| 51 | 4 | | 1.485992 | 1.483110 | 1.491943 | 1.483110 |
| 52 | 3 | | 1.486688 | 1.483062 | 1.491892 | 1.483062 |
| 53 | 4 | | 1.485513 | 1.482974 | 1.491808 | 1.482974 |
| 54 | 4 | 1 | 1.486939 | 1.481321 | 1.490078 | 1.481279 |
| 55 | 2 | | 1.487088 | 1.485237 | 1.494134 | 1.485237 |
| 56 | 3 | | 1.492096 | 1.486999 | 1.495917 | 1.486999 |
| 57 | 2 | | 1.494206 | 1.484773 | 1.493647 | 1.484773 |
| 58 | 6 | | 1.487099 | 1.484089 | 1.492941 | 1.484089 |
| 59 | 2 | | 1.491593 | 1.481931 | 1.490737 | 1.481931 |
| 60 | 2 | | 1.491013 | 1.481462 | 1.490263 | 1.481462 |
| 61 | 4 | | 1.487842 | 1.484769 | 1.493646 | 1.484769 |
| 62 | 6 | | 1.491998 | 1.486881 | 1.495802 | 1.486881 |
| 63 | 4 | 1 | 1.489714 | 1.486381 | 1.454426 | 1.445767 |
| 64 | 4 | | 1.498233 | 1.484538 | 1.493410 | 1.484538 |
| 65 | 2 | | 1.487541 | 1.484280 | 1.493151 | 1.484280 |
| 66 | 4 | | 1.491876 | 1.485023 | 1.493895 | 1.485023 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 67 | 3 | | 1.494723 | 1.484632 | 1.493500 | 1.484632 |
| 68 | 6 | | 1.490505 | 1.486368 | 1.495272 | 1.486368 |
| 69 | 5 | | 1.487017 | 1.484143 | 1.493002 | 1.484143 |
| 70 | 7 | 1 | 1.491892 | 1.485502 | 1.494382 | 1.485499 |
| 71 | 3 | | 1.490005 | 1.484087 | 1.492940 | 1.484087 |
| 72 | 5 | | 1.489044 | 1.484518 | 1.493382 | 1.484518 |
| 73 | 5 | | 1.481098 | 1.485576 | 1.494473 | 1.485576 |
| 74 | 3 | | 1.485907 | 1.485036 | 1.493911 | 1.485036 |
| 75 | 4 | | 1.486212 | 1.487415 | 1.496340 | 1.487415 |
| 76 | 4 | 1 | 1.485839 | 1.487504 | 1.496427 | 1.487504 |
| 77 | 6 | | 1.493681 | 1.479580 | 1.488344 | 1.479580 |
| 78 | 2 | | 1.492457 | 1.485866 | 1.494756 | 1.485866 |
| 79 | 5 | | 1.496172 | 1.480756 | 1.489547 | 1.480756 |
| 80 | 5 | | 1.491701 | 1.486661 | 1.495582 | 1.486661 |
| 81 | 3 | 1 | 1.494453 | 1.483869 | 1.449552 | 1.440955 |
| 82 | 4 | | 1.495608 | 1.486197 | 1.495098 | 1.486197 |
| 83 | 0 | | 1.496437 | 1.482670 | 1.491496 | 1.482670 |
| 84 | 4 | | 1.493455 | 1.484390 | 1.493250 | 1.484390 |
| 85 | 5 | | 1.492077 | 1.484060 | 1.492920 | 1.484060 |
| 86 | 7 | 2 | 1.495684 | 1.481434 | 1.483299 | 1.474542 |
| 87 | 6 | | 1.491491 | 1.485241 | 1.494128 | 1.485241 |
| 88 | 2 | | 1.490886 | 1.486408 | 1.495308 | 1.486408 |
| 89 | 5 | | 1.488840 | 1.491135 | 1.500157 | 1.491135 |
| 90 | 2 | | 1.490806 | 1.487562 | 1.496487 | 1.487562 |
| 91 | 4 | | 1.486625 | 1.483561 | 1.492405 | 1.483561 |
| 92 | 3 | | 1.489903 | 1.483930 | 1.492786 | 1.483930 |
| 93 | 6 | | 1.489295 | 1.481279 | 1.490073 | 1.481279 |
| 94 | 1 | | 1.487901 | 1.486953 | 1.495864 | 1.486953 |
| 95 | 2 | | 1.492588 | 1.482943 | 1.491782 | 1.482943 |
| 96 | 4 | | 1.491244 | 1.487363 | 1.496284 | 1.487363 |
| 97 | 3 | | 1.484455 | 1.484213 | 1.493084 | 1.484213 |
| 98 | 4 | | 1.487070 | 1.482765 | 1.491601 | 1.482765 |
| 99 | 4 | | 1.487673 | 1.482491 | 1.491311 | 1.482492 |
| 100 | 4 | | 1.485230 | 1.482251 | 1.491066 | 1.482251 |
| 101 | 3 | | 1.496313 | 1.476950 | 1.484323 | 1.475622 |
| 102 | 5 | | 1.489723 | 1.480754 | 1.489546 | 1.480754 |
| 103 | 5 | | 1.494842 | 1.480530 | 1.489312 | 1.480530 |
| 104 | 4 | | 1.494518 | 1.485157 | 1.494034 | 1.485157 |
| 105 | 5 | | 1.492956 | 1.483393 | 1.492251 | 1.483393 |
| 106 | 4 | | 1.493801 | 1.483806 | 1.492662 | 1.483806 |

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|---|---|---|---|---|---|---|
| 107 | 5 | 3 | 1.492183 | 1.486141 | 1.495041 | 1.486141 |
| 108 | 4 | 2 | 1.489054 | 1.480472 | 1.489251 | 1.480472 |
| 109 | 3 | 1 | 1.493281 | 1.482596 | 1.491427 | 1.482596 |
| 110 | 4 | | 1.466119 | 1.481285 | 1.460314 | 1.451688 |
| 111 | 3 | | 1.492510 | 1.481746 | 1.490570 | 1.481746 |
| 112 | 4 | | 1.486766 | 1.481283 | 1.490085 | 1.481283 |
| 113 | 3 | | 1.492626 | 1.477860 | 1.486591 | 1.477860 |
| 114 | 3 | | 1.496775 | 1.481169 | 1.489969 | 1.481169 |
| 115 | 4 | | 1.492029 | 1.479133 | 1.487888 | 1.479133 |
| 116 | 4 | | 1.490324 | 1.479830 | 1.488601 | 1.479830 |
| 117 | 4 | | 1.494075 | 1.479665 | 1.488431 | 1.479665 |
| 118 | 4 | | 1.489362 | 1.481758 | 1.490577 | 1.481758 |
| 119 | 3 | 19 | 1.492273 | 1.486041 | 1.494932 | 1.486041 |
| 120 | 4 | | 1.487171 | 1.481686 | 1.490488 | 1.481686 |
| 121 | 4 | | 1.494071 | 1.483647 | 1.492495 | 1.483647 |
| 122 | 3 | 1 | 1.490257 | 1.479170 | 1.487931 | 1.479170 |
| 123 | 5 | 1 | 1.490685 | 1.484487 | 1.493347 | 1.484487 |
| 124 | 5 | 1 | 1.488069 | 1.481466 | 1.490192 | 1.481382 |
| 125 | 4 | | 1.495560 | 1.486113 | 1.495011 | 1.486113 |
| 126 | 4 | | 1.489303 | 1.481424 | 1.490232 | 1.481424 |
| 127 | 5 | 1 | 1.488606 | 1.479715 | 1.488479 | 1.479716 |
| 128 | 4 | | 1.489692 | 1.480578 | 1.489360 | 1.480578 |
| 129 | 4 | | 1.494537 | 1.482709 | 1.491543 | 1.482709 |
| 130 | 4 | 1 | 1.493517 | 1.483985 | 1.492838 | 1.483985 |
| 131 | 5 | | 1.495970 | 1.479197 | 1.487960 | 1.479197 |
| 132 | 5 | 1 | 1.490813 | 1.473060 | 1.481694 | 1.473060 |
| 133 | 4 | 2 | 1.491939 | 1.481517 | 1.490343 | 1.481517 |
| 134 | 4 | | 1.489765 | 1.484061 | 1.492925 | 1.484061 |
| 135 | 3 | | 1.493281 | 1.481590 | 1.490406 | 1.481590 |
| 136 | 4 | 1 | 1.493418 | 1.482391 | 1.491229 | 1.482391 |
| 137 | 2 | | 1.493492 | 1.484327 | 1.479866 | 1.471073 |
| 138 | 4 | 2 | 1.489625 | 1.481384 | 1.490195 | 1.481384 |
| 139 | 3 | | 1.491064 | 1.482341 | 1.491176 | 1.482341 |
| 140 | 3 | | 1.491790 | 1.479283 | 1.488048 | 1.479283 |
| 141 | 5 | | 1.490785 | 1.479229 | 1.488002 | 1.479229 |
| 142 | 4 | | 1.487659 | 1.480936 | 1.489745 | 1.480936 |
| 143 | 5 | | 1.491096 | 1.478885 | 1.487639 | 1.478885 |
| 144 | 4 | | 1.493029 | 1.481845 | 1.490662 | 1.481845 |
| 145 | 5 | | 1.489378 | 1.481928 | 1.490754 | 1.481928 |
| 146 | 5 | | 1.493292 | 1.480773 | 1.489568 | 1.480773 |

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|---|---|---|---|---|---|---|
| 147 | 5 | 1 | 1.493024 | 1.481661 | 1.487639 | 1.478839 |
| 148 | 5 | | 1.493128 | 1.482229 | 1.491059 | 1.482228 |
| 149 | 4 | | 1.492060 | 1.484109 | 1.492961 | 1.484109 |
| 150 | 4 | | 1.492458 | 1.479626 | 1.484683 | 1.475935 |
| 151 | 4 | | 1.491943 | 1.477271 | 1.452740 | 1.444214 |
| 152 | 5 | | 1.491892 | 1.477952 | 1.486688 | 1.477952 |
| 153 | 3 | | 1.491808 | 1.476801 | 1.485513 | 1.476801 |
| 154 | 4 | | 1.490120 | 1.478195 | 1.486939 | 1.478195 |
| 155 | 5 | | 1.494134 | 1.478340 | 1.487088 | 1.478340 |
| 156 | 6 | 1 | 1.495917 | 1.483243 | 1.492096 | 1.483243 |
| 157 | 5 | | 1.493647 | 1.485315 | 1.494206 | 1.485315 |
| 158 | 5 | | 1.492941 | 1.478347 | 1.487099 | 1.478347 |
| 159 | 5 | | 1.490737 | 1.482753 | 1.491593 | 1.482753 |
| 160 | 4 | | 1.490263 | 1.482190 | 1.491013 | 1.482190 |
| 161 | 4 | | 1.493646 | 1.479083 | 1.487842 | 1.479083 |
| 162 | 6 | 1 | 1.495802 | 1.483155 | 1.489466 | 1.480638 |
| 163 | 5 | | 1.495283 | 1.480911 | 1.489714 | 1.480911 |
| 164 | 6 | | 1.493410 | 1.489267 | 1.498233 | 1.489267 |
| 165 | 5 | | 1.493151 | 1.478785 | 1.487541 | 1.478785 |
| 166 | 6 | | 1.493894 | 1.483036 | 1.491876 | 1.483036 |
| 167 | 5 | 3 | 1.493500 | 1.485819 | 1.483702 | 1.474864 |
| 168 | 6 | 1 | 1.495272 | 1.481693 | 1.490505 | 1.481693 |
| 169 | 5 | | 1.493002 | 1.478274 | 1.487017 | 1.478273 |
| 170 | 6 | 1 | 1.494384 | 1.483056 | 1.479295 | 1.470534 |
| 171 | 6 | | 1.492940 | 1.481199 | 1.490005 | 1.481199 |
| 172 | 5 | | 1.493382 | 1.480257 | 1.489044 | 1.480257 |
| 173 | 5 | 2 | 1.494473 | 1.472474 | 1.481098 | 1.472474 |
| 174 | 4 | | 1.493911 | 1.477187 | 1.485907 | 1.477187 |
| 175 | 4 | | 1.496340 | 1.477490 | 1.486158 | 1.477436 |
| 176 | 4 | 1 | 1.496427 | 1.477120 | 1.485839 | 1.477120 |
| 177 | 5 | | 1.488345 | 1.484797 | 1.493680 | 1.484796 |
| 178 | 5 | | 1.494756 | 1.483607 | 1.492457 | 1.483607 |
| 179 | 3 | | 1.489547 | 1.487243 | 1.496172 | 1.487243 |
| 180 | 4 | | 1.495582 | 1.482864 | 1.491688 | 1.482851 |
| 181 | 3 | | 1.492722 | 1.485568 | 1.494453 | 1.485568 |
| 182 | 3 | | 1.495098 | 1.486703 | 1.495608 | 1.486703 |
| 183 | 4 | | 1.491496 | 1.487506 | 1.496424 | 1.487493 |
| 184 | 3 | | 1.493250 | 1.484575 | 1.493455 | 1.484575 |
| 185 | 6 | | 1.492920 | 1.483225 | 1.492077 | 1.483225 |
| 186 | 6 | | 1.490232 | 1.486766 | 1.495684 | 1.486766 |

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|---|---|---|---|---|---|
| 187 | 4 | 1.494128 | 1.482665 | 1.491491 | 1.482665 |
| 188 | 5 | 1.495308 | 1.482067 | 1.490886 | 1.482067 |
| 189 | 5 | 1.500157 | 1.480061 | 1.488840 | 1.480061 |
| 190 | 4 | 1.496487 | 1.481981 | 1.490806 | 1.481981 |
| 191 | 4 | 1.492405 | 1.477892 | 1.455883 | 1.447331 |
| 192 | 4 | 1.492786 | 1.481102 | 1.489904 | 1.481102 |
| 193 | 5 | 1.490073 | 1.480501 | 1.489294 | 1.480501 |
| 194 | 3 | 1.495864 | 1.479148 | 1.487901 | 1.479148 |
| 195 | 3 | 1.491782 | 1.483725 | 1.492588 | 1.483725 |
| 196 | 3 | 1.496284 | 1.482415 | 1.491244 | 1.482415 |
| 197 | 4 | 1.493084 | 1.475771 | 1.484455 | 1.475771 |
| 198 | 5 | 1.491601 | 1.478331 | 1.487070 | 1.478331 |
| 199 | 5 | 1.491311 | 1.478918 | 1.469607 | 1.460958 |
| 200 | 4 | 1.491066 | 1.476528 | 1.485230 | 1.476528 |

## β-$D_3$/β-$H_3$ isotopic partition-function ratios for ($NC^{-}\cdots EtCl$).*n*DMSO reactant structures:

| structure sequence number | *n* | number extra imaginaries | extra imaginaries treated as reals: 300 K $f_{RS}$ | extra imaginaries treated as reals: 303.15K $f_{RS}$ | extra imaginaries omitted: 300 K $f_{RS}$ | extra imaginaries omitted: 303.15K $f_{RS}$ |
|---|---|---|---|---|---|---|
| 1 | 4 | | 1816.146484 | 1632.392700 | 1805.446777 | 1632.392944 |
| 2 | 5 | 1 | 1829.145752 | 1643.610474 | 1766.000000 | 1596.779663 |
| 3 | 4 | | 1849.433838 | 1673.411377 | 1851.555664 | 1673.411377 |
| 4 | 4 | | 1898.890137 | 1688.045532 | 1867.604004 | 1688.045532 |
| 5 | 4 | | 1837.795898 | 1666.448975 | 1843.587769 | 1666.448975 |
| 6 | 7 | | 1864.273682 | 1635.368652 | 1808.987671 | 1635.368530 |
| 7 | 3 | | 1860.055054 | 1687.562012 | 1867.167236 | 1687.562012 |
| 8 | 6 | 1 | 1853.967407 | 1643.359741 | 1818.014404 | 1643.354492 |
| 9 | 5 | | 1861.541870 | 1665.907837 | 1843.073486 | 1665.907837 |
| 10 | 1 | 10 | 1828.223755 | 1485.596313 | 1512.629150 | 1368.797607 |
| 11 | 4 | 1 | 1833.292114 | 1701.884521 | 1883.257690 | 1701.838501 |
| 12 | 3 | | 1847.828979 | 1650.487061 | 1826.038574 | 1650.487183 |
| 13 | 4 | | 1834.366821 | 1667.444458 | 1844.636719 | 1667.444946 |
| 14 | 5 | | 1834.269043 | 1671.647339 | 1849.437134 | 1671.647339 |
| 15 | 5 | | 1861.102783 | 1670.680908 | 1848.115112 | 1670.680908 |
| 16 | 4 | 2 | 1813.257935 | 1682.442139 | 1814.354004 | 1639.927124 |
| 17 | 7 | 1 | 1848.263672 | 1654.454468 | 1828.895630 | 1653.390259 |
| 18 | 5 | | 1854.676758 | 1673.359985 | 1851.300781 | 1673.359863 |
| 19 | 3 | | 1864.107422 | 1698.096313 | 1878.989014 | 1698.096313 |
| 20 | 2 | | 1829.285278 | 1673.126465 | 1850.847778 | 1673.126465 |
| 21 | 3 | | 1810.458862 | 1682.432007 | 1861.446777 | 1682.432007 |
| 22 | 5 | | 1829.140259 | 1708.909424 | 1891.178223 | 1708.909424 |
| 23 | 2 | | 1878.046021 | 1715.537476 | 1898.615723 | 1715.537476 |
| 24 | 4 | | 1823.902588 | 1661.129639 | 1837.796509 | 1661.129639 |
| 25 | 3 | | 1924.818848 | 1694.475098 | 1874.857422 | 1694.475098 |
| 26 | 5 | | 1838.996216 | 1655.973022 | 1832.069458 | 1655.972900 |

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|---|---|---|---|---|---|---|
| 27 | 6 | | 1836.555176 | 1642.178711 | 1816.537720 | 1642.177734 |
| 28 | 5 | | 1829.402832 | 1649.294678 | 1824.475708 | 1649.294678 |
| 29 | 6 | | 1827.894287 | 1656.967896 | 1832.790527 | 1656.967407 |
| 30 | 5 | 1 | 1862.466187 | 1636.222900 | 1782.047241 | 1611.164185 |
| 31 | 4 | | 1842.494873 | 1688.743042 | 1868.450684 | 1688.743286 |
| 32 | 3 | | 1819.875488 | 1640.556152 | 1814.613647 | 1640.556152 |
| 33 | 2 | | 1825.720459 | 1642.536743 | 1816.739258 | 1642.536743 |
| 34 | 5 | | 1829.656494 | 1672.090942 | 1849.715088 | 1672.090942 |
| 35 | 6 | | 1831.388672 | 1662.140991 | 1838.714844 | 1662.140991 |
| 36 | 6 | | 1803.693115 | 1678.568481 | 1857.085571 | 1678.568481 |
| 37 | 5 | | 1828.456055 | 1668.716431 | 1846.045654 | 1668.716431 |
| 38 | 5 | | 1837.378296 | 1675.380005 | 1853.497681 | 1675.380005 |
| 39 | 4 | | 1841.353638 | 1671.145142 | 1848.719849 | 1671.145142 |
| 40 | 5 | 1 | 1817.239624 | 1664.989990 | 1837.284058 | 1660.850830 |
| 41 | 5 | | 1819.646606 | 1651.404419 | 1826.591187 | 1651.404541 |
| 42 | 4 | | 1864.914795 | 1709.855835 | 1892.260742 | 1709.855713 |
| 43 | 2 | | 1836.147583 | 1733.708130 | 1918.814575 | 1733.708130 |
| 44 | 6 | | 1808.925293 | 1696.546387 | 1877.201904 | 1696.546387 |
| 45 | 5 | 1 | 1824.726685 | 1721.254761 | 1902.193726 | 1718.650269 |
| 46 | 4 | | 1808.703369 | 1697.338257 | 1878.004639 | 1697.338257 |
| 47 | 4 | 1 | 1838.550537 | 1634.991699 | 1807.932739 | 1634.720581 |
| 48 | 3 | | 1846.363403 | 1666.102295 | 1843.027100 | 1666.102417 |
| 49 | 4 | | 1851.685669 | 1688.957153 | 1868.585449 | 1688.957031 |
| 50 | 4 | | 1836.891724 | 1681.664429 | 1860.482422 | 1681.664429 |
| 51 | 4 | | 1775.258179 | 1629.641968 | 1802.481079 | 1629.641968 |
| 52 | 3 | | 1827.602173 | 1630.962891 | 1803.854980 | 1630.962891 |
| 53 | 4 | | 1802.556152 | 1658.449585 | 1834.440430 | 1658.449585 |
| 54 | 4 | 1 | 1821.580688 | 1668.204102 | 1845.534912 | 1668.130615 |
| 55 | 2 | | 1819.047241 | 1690.671875 | 1870.591919 | 1690.671875 |
| 56 | 3 | | 1807.854736 | 1700.827637 | 1882.072144 | 1700.827759 |
| 57 | 2 | | 1818.426514 | 1681.773071 | 1860.601685 | 1681.773193 |
| 58 | 6 | | 1828.040161 | 1680.793457 | 1859.688843 | 1680.793457 |
| 59 | 2 | | 1842.206299 | 1695.293823 | 1875.719604 | 1695.293823 |
| 60 | 2 | | 1816.738037 | 1659.898315 | 1836.066528 | 1659.898315 |
| 61 | 4 | | 1820.907471 | 1668.812744 | 1846.248413 | 1668.812866 |
| 62 | 6 | | 1808.409058 | 1672.082520 | 1849.682373 | 1672.082642 |
| 63 | 4 | 1 | 1807.900513 | 1641.195923 | 1785.979858 | 1614.731567 |
| 64 | 4 | | 1809.078247 | 1648.097412 | 1823.041260 | 1648.097412 |
| 65 | 2 | | 1820.642456 | 1713.547485 | 1896.306396 | 1713.547485 |
| 66 | 4 | | 1874.463745 | 1675.516113 | 1853.565674 | 1675.516235 |

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|---|---|---|---|---|---|---|
| 67 | 3 | | 1824.188232 | 1710.936768 | 1893.348999 | 1710.936768 |
| 68 | 6 | | 1850.995117 | 1695.206787 | 1875.749634 | 1695.206787 |
| 69 | 5 | | 1802.957031 | 1677.201904 | 1855.463257 | 1677.202026 |
| 70 | 7 | 1 | 1847.588379 | 1660.190308 | 1836.517700 | 1660.185913 |
| 71 | 3 | | 1814.329468 | 1656.012451 | 1831.806396 | 1656.012451 |
| 72 | 5 | | 1803.203857 | 1679.094482 | 1857.634277 | 1679.094482 |
| 73 | 5 | | 1824.457886 | 1660.074585 | 1836.284302 | 1660.074585 |
| 74 | 3 | | 1799.848999 | 1693.653809 | 1873.909790 | 1693.653809 |
| 75 | 4 | | 1831.188110 | 1665.465210 | 1842.268799 | 1665.465210 |
| 76 | 4 | 1 | 1804.912231 | 1660.172607 | 1836.484253 | 1660.171021 |
| 77 | 6 | | 1822.101685 | 1641.742554 | 1815.827759 | 1641.742554 |
| 78 | 2 | | 1823.282471 | 1655.427002 | 1831.290649 | 1655.427002 |
| 79 | 5 | | 1873.289673 | 1663.803223 | 1840.645630 | 1663.803101 |
| 80 | 5 | | 1851.673218 | 1672.321289 | 1850.031372 | 1672.321289 |
| 81 | 3 | 1 | 1843.345947 | 1694.665283 | 1752.516968 | 1583.917603 |
| 82 | 4 | | 1836.276611 | 1642.056030 | 1816.245239 | 1642.056030 |
| 83 | 0 | | 1847.901978 | 1694.452026 | 1874.807983 | 1694.452026 |
| 84 | 4 | | 1816.201294 | 1650.622437 | 1825.832520 | 1650.622437 |
| 85 | 5 | | 1822.429688 | 1678.234619 | 1856.838013 | 1678.234619 |
| 86 | 7 | 2 | 1819.656006 | 1627.751709 | 1789.091187 | 1617.562866 |
| 87 | 6 | | 1819.678955 | 1668.930420 | 1846.365234 | 1668.930420 |
| 88 | 2 | | 1845.404175 | 1688.522217 | 1868.109985 | 1688.522217 |
| 89 | 5 | | 1822.349243 | 1703.162354 | 1884.673462 | 1703.162354 |
| 90 | 2 | | 1852.906982 | 1748.890381 | 1935.978760 | 1748.890015 |
| 91 | 4 | | 1788.806030 | 1682.121338 | 1861.029663 | 1682.121338 |
| 92 | 3 | | 1816.816528 | 1731.649048 | 1916.644897 | 1731.649048 |
| 93 | 6 | | 1807.261353 | 1680.214233 | 1858.827515 | 1680.214233 |
| 94 | 1 | | 1833.010986 | 1675.353638 | 1853.317505 | 1675.353638 |
| 95 | 2 | | 1862.527100 | 1689.256348 | 1869.029175 | 1689.256348 |
| 96 | 4 | | 1816.293701 | 1691.312378 | 1871.539673 | 1691.312378 |
| 97 | 3 | | 1838.750000 | 1721.769165 | 1905.523071 | 1721.769165 |
| 98 | 4 | | 1816.983276 | 1753.301147 | 1941.224243 | 1753.301025 |
| 99 | 4 | | 1823.266357 | 1690.015381 | 1869.983887 | 1690.015381 |
| 100 | 4 | | 1888.466309 | 1698.734619 | 1879.671997 | 1698.734619 |
| 101 | 3 | | 1805.446533 | 1641.908203 | 1815.715942 | 1641.519165 |
| 102 | 5 | | 1817.793945 | 1653.711792 | 1829.145752 | 1653.711792 |
| 103 | 5 | | 1851.555664 | 1671.786987 | 1849.433838 | 1671.786987 |
| 104 | 4 | | 1867.604004 | 1715.626099 | 1898.890137 | 1715.626099 |
| 105 | 5 | | 1843.587769 | 1661.454102 | 1837.796021 | 1661.454102 |
| 106 | 4 | | 1808.987793 | 1685.007324 | 1864.273682 | 1685.007324 |

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|---|---|---|---|---|---|---|
| 107 | 5 | 3 | 1867.167236 | 1681.197632 | 1860.054932 | 1681.197510 |
| 108 | 4 | 2 | 1818.020142 | 1675.693115 | 1853.967407 | 1675.693115 |
| 109 | 3 | 1 | 1843.073608 | 1682.584229 | 1861.541870 | 1682.584229 |
| 110 | 4 | | 1641.702759 | 1652.904541 | 1701.913696 | 1538.707520 |
| 111 | 3 | | 1883.308716 | 1657.441895 | 1833.292114 | 1657.441895 |
| 112 | 4 | | 1826.038574 | 1670.371704 | 1847.828979 | 1670.371704 |
| 113 | 3 | | 1844.636108 | 1658.269165 | 1834.366821 | 1658.269165 |
| 114 | 3 | | 1849.437134 | 1658.182129 | 1834.269043 | 1658.182129 |
| 115 | 4 | | 1848.115234 | 1682.137695 | 1861.102783 | 1682.137695 |
| 116 | 4 | | 1861.391235 | 1639.476807 | 1813.257935 | 1639.476807 |
| 117 | 4 | | 1830.072876 | 1670.787842 | 1848.263672 | 1670.787842 |
| 118 | 4 | | 1851.300903 | 1676.485352 | 1854.676758 | 1676.485352 |
| 119 | 3 | 19 | 1878.989014 | 1684.936279 | 1864.107422 | 1684.936279 |
| 120 | 4 | | 1850.847778 | 1653.615112 | 1829.285400 | 1653.615234 |
| 121 | 4 | | 1861.446777 | 1636.805176 | 1810.458862 | 1636.805176 |
| 122 | 3 | 1 | 1891.178223 | 1653.754761 | 1829.140259 | 1653.754761 |
| 123 | 5 | 1 | 1898.615723 | 1697.140869 | 1878.046021 | 1697.140869 |
| 124 | 5 | 1 | 1837.796509 | 1648.926392 | 1823.676758 | 1648.722290 |
| 125 | 4 | | 1874.857422 | 1738.880615 | 1924.818848 | 1738.880615 |
| 126 | 4 | | 1832.069580 | 1662.576538 | 1838.996216 | 1662.576538 |
| 127 | 5 | 1 | 1816.538818 | 1660.224731 | 1836.555176 | 1660.224731 |
| 128 | 4 | | 1824.475708 | 1653.853638 | 1829.402832 | 1653.853638 |
| 129 | 4 | | 1832.791016 | 1652.574585 | 1827.894287 | 1652.574585 |
| 130 | 4 | 1 | 1809.763794 | 1683.448120 | 1862.466187 | 1683.448120 |
| 131 | 5 | | 1868.450439 | 1665.675171 | 1842.494873 | 1665.675171 |
| 132 | 5 | 1 | 1814.613647 | 1645.421265 | 1819.875732 | 1645.421509 |
| 133 | 4 | 2 | 1816.739258 | 1650.641113 | 1825.720459 | 1650.640991 |
| 134 | 4 | | 1849.715088 | 1653.974976 | 1829.656494 | 1653.974976 |
| 135 | 3 | | 1838.714844 | 1655.744995 | 1831.388672 | 1655.744995 |
| 136 | 4 | 1 | 1857.085571 | 1630.958008 | 1803.693115 | 1630.958008 |
| 137 | 2 | | 1846.045654 | 1652.929810 | 1803.155518 | 1630.058228 |
| 138 | 4 | 2 | 1853.497681 | 1661.092773 | 1837.378296 | 1661.092773 |
| 139 | 3 | | 1848.719849 | 1664.600342 | 1841.353638 | 1664.600342 |
| 140 | 3 | | 1841.863037 | 1642.888550 | 1817.239624 | 1642.888550 |
| 141 | 5 | | 1826.591187 | 1645.169800 | 1819.646606 | 1645.169800 |
| 142 | 4 | | 1892.260742 | 1685.463989 | 1864.914795 | 1685.463989 |
| 143 | 5 | | 1918.814697 | 1659.783447 | 1836.147583 | 1659.783447 |
| 144 | 4 | | 1877.201904 | 1635.467896 | 1808.925293 | 1635.467896 |
| 145 | 5 | | 1905.076416 | 1649.535889 | 1824.726685 | 1649.535767 |
| 146 | 5 | | 1878.004639 | 1635.335693 | 1808.703369 | 1635.335693 |

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|---|---|---|---|---|---|---|
| 147 | 5 | 1 | 1808.232788 | 1661.761475 | 1835.201172 | 1658.734131 |
| 148 | 5 | | 1843.027100 | 1668.991333 | 1846.363403 | 1668.991333 |
| 149 | 4 | | 1868.585571 | 1673.741821 | 1851.685669 | 1673.741821 |
| 150 | 4 | | 1860.482422 | 1660.500122 | 1834.271118 | 1658.131226 |
| 151 | 4 | | 1802.481079 | 1605.485718 | 1670.665771 | 1510.896362 |
| 152 | 5 | | 1803.855103 | 1652.348633 | 1827.602173 | 1652.348633 |
| 153 | 3 | | 1834.440430 | 1629.808472 | 1802.556152 | 1629.808472 |
| 154 | 4 | | 1845.616211 | 1646.694092 | 1821.580688 | 1646.694092 |
| 155 | 5 | | 1870.591919 | 1644.585449 | 1819.047241 | 1644.585449 |
| 156 | 6 | 1 | 1882.072144 | 1634.556030 | 1807.854736 | 1634.556030 |
| 157 | 5 | | 1860.601685 | 1643.801636 | 1818.426636 | 1643.801636 |
| 158 | 5 | | 1859.688843 | 1652.553955 | 1828.040161 | 1652.553955 |
| 159 | 5 | | 1875.719604 | 1665.218872 | 1842.206299 | 1665.218872 |
| 160 | 4 | | 1836.066528 | 1642.613281 | 1816.738037 | 1642.613281 |
| 161 | 4 | | 1846.248291 | 1646.252930 | 1820.907471 | 1646.252930 |
| 162 | 6 | 1 | 1849.682251 | 1634.879028 | 1805.306396 | 1632.073975 |
| 163 | 5 | | 1815.250977 | 1634.426636 | 1807.900513 | 1634.426636 |
| 164 | 6 | | 1823.041260 | 1635.587158 | 1809.078247 | 1635.587158 |
| 165 | 5 | | 1896.306396 | 1646.073120 | 1820.642456 | 1646.073120 |
| 166 | 6 | | 1853.565552 | 1694.080322 | 1874.463745 | 1694.080322 |
| 167 | 5 | 3 | 1893.348999 | 1648.953979 | 1756.271118 | 1587.561279 |
| 168 | 6 | 1 | 1875.749634 | 1673.114868 | 1850.995117 | 1673.114868 |
| 169 | 5 | | 1855.463135 | 1630.102173 | 1802.957031 | 1630.102173 |
| 170 | 6 | 1 | 1836.522583 | 1669.823486 | 1844.083008 | 1666.655396 |
| 171 | 6 | | 1831.806396 | 1640.365601 | 1814.329468 | 1640.365601 |
| 172 | 5 | | 1857.634277 | 1630.244385 | 1803.203857 | 1630.244385 |
| 173 | 5 | 2 | 1836.284180 | 1649.338867 | 1824.457886 | 1649.338867 |
| 174 | 4 | | 1873.909790 | 1627.305420 | 1799.849121 | 1627.305420 |
| 175 | 4 | | 1842.268799 | 1655.575439 | 1830.909058 | 1655.323120 |
| 176 | 4 | 1 | 1836.485962 | 1631.930176 | 1804.912231 | 1631.930176 |
| 177 | 5 | | 1815.827759 | 1647.354248 | 1822.101563 | 1647.354126 |
| 178 | 5 | | 1831.290649 | 1648.266968 | 1823.282471 | 1648.266968 |
| 179 | 3 | | 1840.645752 | 1692.964478 | 1873.289673 | 1692.964478 |
| 180 | 4 | | 1850.031372 | 1673.813721 | 1851.452759 | 1673.614502 |
| 181 | 3 | | 1875.053345 | 1666.383545 | 1843.345947 | 1666.383545 |
| 182 | 3 | | 1816.245239 | 1659.999634 | 1836.276733 | 1659.999878 |
| 183 | 4 | | 1874.807983 | 1670.167603 | 1847.887085 | 1670.154175 |
| 184 | 3 | | 1825.832520 | 1642.065063 | 1816.201538 | 1642.065308 |
| 185 | 6 | | 1856.838013 | 1647.323364 | 1822.429688 | 1647.323242 |
| 186 | 6 | | 1800.360718 | 1644.985962 | 1819.656006 | 1644.985962 |

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|---|---|---|---|---|---|
| 187 | 4 | 1846.365234 | 1645.067993 | 1819.679077 | 1645.067993 |
| 188 | 5 | 1868.109985 | 1668.205444 | 1845.404175 | 1668.205322 |
| 189 | 5 | 1884.673462 | 1647.653198 | 1822.349243 | 1647.653198 |
| 190 | 4 | 1935.979126 | 1674.962891 | 1852.906982 | 1674.962891 |
| 191 | 4 | 1861.029663 | 1617.401001 | 1719.564819 | 1554.794678 |
| 192 | 4 | 1916.644897 | 1642.538940 | 1816.816650 | 1642.539063 |
| 193 | 5 | 1858.827515 | 1634.001343 | 1807.261353 | 1634.001343 |
| 194 | 3 | 1853.317505 | 1656.979980 | 1833.010986 | 1656.979980 |
| 195 | 3 | 1869.029175 | 1683.320313 | 1862.526978 | 1683.320313 |
| 196 | 3 | 1871.539673 | 1642.019775 | 1816.293701 | 1642.019775 |
| 197 | 4 | 1905.523071 | 1662.090210 | 1838.749878 | 1662.090088 |
| 198 | 5 | 1941.224365 | 1642.681030 | 1816.983276 | 1642.681030 |
| 199 | 5 | 1869.983887 | 1648.409668 | 1772.750732 | 1602.738892 |
| 200 | 4 | 1879.671875 | 1706.346802 | 1888.466309 | 1706.346802 |

## $\alpha$-$^{14}$C/$\alpha$-$^{11}$C isotopic partition-function ratios for (NC$^{-}$···EtCl).*n*DMSO reactant structures:

| structure sequence number | *n* | number extra imaginaries | extra imaginaries treated as reals | | extra imaginaries omitted | |
|---|---|---|---|---|---|---|
| | | | 300 K | 303.15K | 300 K | 303.15K |
| | | | $f_{RS}$ | $f_{RS}$ | $f_{RS}$ | $f_{RS}$ |
| 1 | 4 | | 1.485658 | 1.487392 | 1.496313 | 1.487392 |
| 2 | 5 | 1 | 1.489546 | 1.480933 | 1.466005 | 1.457355 |
| 3 | 4 | | 1.489312 | 1.485943 | 1.494842 | 1.485943 |
| 4 | 4 | | 1.494034 | 1.485614 | 1.494518 | 1.485614 |
| 5 | 4 | | 1.492251 | 1.484102 | 1.492956 | 1.484102 |
| 6 | 7 | | 1.492662 | 1.484928 | 1.493801 | 1.484928 |
| 7 | 3 | | 1.495041 | 1.483348 | 1.492183 | 1.483348 |
| 8 | 6 | 1 | 1.489251 | 1.480280 | 1.489054 | 1.480280 |
| 9 | 5 | | 1.491427 | 1.484418 | 1.493281 | 1.484418 |
| 10 | 1 | 10 | 1.490087 | 1.457695 | 1.389013 | 1.381033 |
| 11 | 4 | 1 | 1.490570 | 1.483660 | 1.492465 | 1.483616 |
| 12 | 3 | | 1.490085 | 1.478033 | 1.486766 | 1.478033 |
| 13 | 4 | | 1.486591 | 1.483775 | 1.492627 | 1.483775 |
| 14 | 5 | | 1.489969 | 1.487842 | 1.496775 | 1.487842 |
| 15 | 5 | | 1.487888 | 1.483187 | 1.492029 | 1.483187 |
| 16 | 4 | 2 | 1.488601 | 1.481520 | 1.453649 | 1.445061 |
| 17 | 7 | 1 | 1.488431 | 1.485199 | 1.493392 | 1.484520 |
| 18 | 5 | | 1.490577 | 1.480582 | 1.489362 | 1.480583 |
| 19 | 3 | | 1.494932 | 1.483431 | 1.492273 | 1.483431 |
| 20 | 2 | | 1.490487 | 1.478435 | 1.487171 | 1.478435 |
| 21 | 3 | | 1.492495 | 1.485187 | 1.494071 | 1.485187 |
| 22 | 5 | | 1.487931 | 1.481461 | 1.490257 | 1.481461 |
| 23 | 2 | | 1.493347 | 1.481878 | 1.490685 | 1.481878 |
| 24 | 4 | | 1.490277 | 1.479312 | 1.488069 | 1.479312 |
| 25 | 3 | | 1.495011 | 1.486655 | 1.495560 | 1.486655 |
| 26 | 5 | | 1.490232 | 1.480524 | 1.489303 | 1.480524 |

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|---|---|---|---|---|---|---|
| 27 | 6 | | 1.488479 | 1.479836 | 1.488606 | 1.479836 |
| 28 | 5 | | 1.489360 | 1.480901 | 1.489692 | 1.480901 |
| 29 | 6 | | 1.491543 | 1.485622 | 1.494538 | 1.485623 |
| 30 | 5 | 1 | 1.492838 | 1.484653 | 1.471887 | 1.463152 |
| 31 | 4 | | 1.487960 | 1.487058 | 1.495970 | 1.487058 |
| 32 | 3 | | 1.481694 | 1.482000 | 1.490813 | 1.482000 |
| 33 | 2 | | 1.490343 | 1.483105 | 1.491939 | 1.483105 |
| 34 | 5 | | 1.492925 | 1.480974 | 1.489765 | 1.480974 |
| 35 | 6 | | 1.490406 | 1.484410 | 1.493281 | 1.484410 |
| 36 | 6 | | 1.491229 | 1.484540 | 1.493418 | 1.484541 |
| 37 | 5 | | 1.493200 | 1.484620 | 1.493492 | 1.484620 |
| 38 | 5 | | 1.490195 | 1.480829 | 1.489625 | 1.480829 |
| 39 | 4 | | 1.491176 | 1.482250 | 1.491064 | 1.482250 |
| 40 | 5 | 1 | 1.488048 | 1.482946 | 1.489022 | 1.480194 |
| 41 | 5 | | 1.488002 | 1.481975 | 1.490785 | 1.481975 |
| 42 | 4 | | 1.489745 | 1.478909 | 1.487659 | 1.478909 |
| 43 | 2 | | 1.487639 | 1.482276 | 1.491096 | 1.482276 |
| 44 | 6 | | 1.490662 | 1.484164 | 1.493029 | 1.484164 |
| 45 | 5 | 1 | 1.490754 | 1.480592 | 1.485975 | 1.477208 |
| 46 | 4 | | 1.489568 | 1.484434 | 1.493292 | 1.484434 |
| 47 | 4 | 1 | 1.490479 | 1.484164 | 1.492985 | 1.484124 |
| 48 | 3 | | 1.491059 | 1.484271 | 1.493128 | 1.484271 |
| 49 | 4 | | 1.492961 | 1.483226 | 1.492060 | 1.483226 |
| 50 | 4 | | 1.488396 | 1.483608 | 1.492458 | 1.483608 |
| 51 | 4 | | 1.485992 | 1.483110 | 1.491943 | 1.483110 |
| 52 | 3 | | 1.486688 | 1.483062 | 1.491892 | 1.483062 |
| 53 | 4 | | 1.485513 | 1.482974 | 1.491808 | 1.482974 |
| 54 | 4 | 1 | 1.486939 | 1.481321 | 1.490078 | 1.481279 |
| 55 | 2 | | 1.487088 | 1.485237 | 1.494134 | 1.485237 |
| 56 | 3 | | 1.492096 | 1.486999 | 1.495917 | 1.486999 |
| 57 | 2 | | 1.494206 | 1.484773 | 1.493647 | 1.484773 |
| 58 | 6 | | 1.487099 | 1.484089 | 1.492941 | 1.484089 |
| 59 | 2 | | 1.491593 | 1.481931 | 1.490737 | 1.481931 |
| 60 | 2 | | 1.491013 | 1.481462 | 1.490263 | 1.481462 |
| 61 | 4 | | 1.487842 | 1.484769 | 1.493646 | 1.484769 |
| 62 | 6 | | 1.491998 | 1.486881 | 1.495802 | 1.486881 |
| 63 | 4 | 1 | 1.489714 | 1.486381 | 1.454426 | 1.445767 |
| 64 | 4 | | 1.498233 | 1.484538 | 1.493410 | 1.484538 |
| 65 | 2 | | 1.487541 | 1.484280 | 1.493151 | 1.484280 |
| 66 | 4 | | 1.491876 | 1.485023 | 1.493895 | 1.485023 |

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|---|---|---|---|---|---|---|
| 67 | 3 | | 1.494723 | 1.484632 | 1.493500 | 1.484632 |
| 68 | 6 | | 1.490505 | 1.486368 | 1.495272 | 1.486368 |
| 69 | 5 | | 1.487017 | 1.484143 | 1.493002 | 1.484143 |
| 70 | 7 | 1 | 1.491892 | 1.485502 | 1.494382 | 1.485499 |
| 71 | 3 | | 1.490005 | 1.484087 | 1.492940 | 1.484087 |
| 72 | 5 | | 1.489044 | 1.484518 | 1.493382 | 1.484518 |
| 73 | 5 | | 1.481098 | 1.485576 | 1.494473 | 1.485576 |
| 74 | 3 | | 1.485907 | 1.485036 | 1.493911 | 1.485036 |
| 75 | 4 | | 1.486212 | 1.487415 | 1.496340 | 1.487415 |
| 76 | 4 | 1 | 1.485839 | 1.487504 | 1.496427 | 1.487504 |
| 77 | 6 | | 1.493681 | 1.479580 | 1.488344 | 1.479580 |
| 78 | 2 | | 1.492457 | 1.485866 | 1.494756 | 1.485866 |
| 79 | 5 | | 1.496172 | 1.480756 | 1.489547 | 1.480756 |
| 80 | 5 | | 1.491701 | 1.486661 | 1.495582 | 1.486661 |
| 81 | 3 | 1 | 1.494453 | 1.483869 | 1.449552 | 1.440955 |
| 82 | 4 | | 1.495608 | 1.486197 | 1.495098 | 1.486197 |
| 83 | 0 | | 1.496437 | 1.482670 | 1.491496 | 1.482670 |
| 84 | 4 | | 1.493455 | 1.484390 | 1.493250 | 1.484390 |
| 85 | 5 | | 1.492077 | 1.484060 | 1.492920 | 1.484060 |
| 86 | 7 | 2 | 1.495684 | 1.481434 | 1.483299 | 1.474542 |
| 87 | 6 | | 1.491491 | 1.485241 | 1.494128 | 1.485241 |
| 88 | 2 | | 1.490886 | 1.486408 | 1.495308 | 1.486408 |
| 89 | 5 | | 1.488840 | 1.491135 | 1.500157 | 1.491135 |
| 90 | 2 | | 1.490806 | 1.487562 | 1.496487 | 1.487562 |
| 91 | 4 | | 1.486625 | 1.483561 | 1.492405 | 1.483561 |
| 92 | 3 | | 1.489903 | 1.483930 | 1.492786 | 1.483930 |
| 93 | 6 | | 1.489295 | 1.481279 | 1.490073 | 1.481279 |
| 94 | 1 | | 1.487901 | 1.486953 | 1.495864 | 1.486953 |
| 95 | 2 | | 1.492588 | 1.482943 | 1.491782 | 1.482943 |
| 96 | 4 | | 1.491244 | 1.487363 | 1.496284 | 1.487363 |
| 97 | 3 | | 1.484455 | 1.484213 | 1.493084 | 1.484213 |
| 98 | 4 | | 1.487070 | 1.482765 | 1.491601 | 1.482765 |
| 99 | 4 | | 1.487673 | 1.482491 | 1.491311 | 1.482492 |
| 100 | 4 | | 1.485230 | 1.482251 | 1.491066 | 1.482251 |
| 101 | 3 | | 1.496313 | 1.476950 | 1.484323 | 1.475622 |
| 102 | 5 | | 1.489723 | 1.480754 | 1.489546 | 1.480754 |
| 103 | 5 | | 1.494842 | 1.480530 | 1.489312 | 1.480530 |
| 104 | 4 | | 1.494518 | 1.485157 | 1.494034 | 1.485157 |
| 105 | 5 | | 1.492956 | 1.483393 | 1.492251 | 1.483393 |
| 106 | 4 | | 1.493801 | 1.483806 | 1.492662 | 1.483806 |

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|---|---|---|---|---|---|---|
| 107 | 5 | 3 | 1.492183 | 1.486141 | 1.495041 | 1.486141 |
| 108 | 4 | 2 | 1.489054 | 1.480472 | 1.489251 | 1.480472 |
| 109 | 3 | 1 | 1.493281 | 1.482596 | 1.491427 | 1.482596 |
| 110 | 4 | | 1.466119 | 1.481285 | 1.460314 | 1.451688 |
| 111 | 3 | | 1.492510 | 1.481746 | 1.490570 | 1.481746 |
| 112 | 4 | | 1.486766 | 1.481283 | 1.490085 | 1.481283 |
| 113 | 3 | | 1.492626 | 1.477860 | 1.486591 | 1.477860 |
| 114 | 3 | | 1.496775 | 1.481169 | 1.489969 | 1.481169 |
| 115 | 4 | | 1.492029 | 1.479133 | 1.487888 | 1.479133 |
| 116 | 4 | | 1.490324 | 1.479830 | 1.488601 | 1.479830 |
| 117 | 4 | | 1.494075 | 1.479665 | 1.488431 | 1.479665 |
| 118 | 4 | | 1.489362 | 1.481758 | 1.490577 | 1.481758 |
| 119 | 3 | 19 | 1.492273 | 1.486041 | 1.494932 | 1.486041 |
| 120 | 4 | | 1.487171 | 1.481686 | 1.490488 | 1.481686 |
| 121 | 4 | | 1.494071 | 1.483647 | 1.492495 | 1.483647 |
| 122 | 3 | 1 | 1.490257 | 1.479170 | 1.487931 | 1.479170 |
| 123 | 5 | 1 | 1.490685 | 1.484487 | 1.493347 | 1.484487 |
| 124 | 5 | 1 | 1.488069 | 1.481466 | 1.490192 | 1.481382 |
| 125 | 4 | | 1.495560 | 1.486113 | 1.495011 | 1.486113 |
| 126 | 4 | | 1.489303 | 1.481424 | 1.490232 | 1.481424 |
| 127 | 5 | 1 | 1.488606 | 1.479715 | 1.488479 | 1.479716 |
| 128 | 4 | | 1.489692 | 1.480578 | 1.489360 | 1.480578 |
| 129 | 4 | | 1.494537 | 1.482709 | 1.491543 | 1.482709 |
| 130 | 4 | 1 | 1.493517 | 1.483985 | 1.492838 | 1.483985 |
| 131 | 5 | | 1.495970 | 1.479197 | 1.487960 | 1.479197 |
| 132 | 5 | 1 | 1.490813 | 1.473060 | 1.481694 | 1.473060 |
| 133 | 4 | 2 | 1.491939 | 1.481517 | 1.490343 | 1.481517 |
| 134 | 4 | | 1.489765 | 1.484061 | 1.492925 | 1.484061 |
| 135 | 3 | | 1.493281 | 1.481590 | 1.490406 | 1.481590 |
| 136 | 4 | 1 | 1.493418 | 1.482391 | 1.491229 | 1.482391 |
| 137 | 2 | | 1.493492 | 1.484327 | 1.479866 | 1.471073 |
| 138 | 4 | 2 | 1.489625 | 1.481384 | 1.490195 | 1.481384 |
| 139 | 3 | | 1.491064 | 1.482341 | 1.491176 | 1.482341 |
| 140 | 3 | | 1.491790 | 1.479283 | 1.488048 | 1.479283 |
| 141 | 5 | | 1.490785 | 1.479229 | 1.488002 | 1.479229 |
| 142 | 4 | | 1.487659 | 1.480936 | 1.489745 | 1.480936 |
| 143 | 5 | | 1.491096 | 1.478885 | 1.487639 | 1.478885 |
| 144 | 4 | | 1.493029 | 1.481845 | 1.490662 | 1.481845 |
| 145 | 5 | | 1.489378 | 1.481928 | 1.490754 | 1.481928 |
| 146 | 5 | | 1.493292 | 1.480773 | 1.489568 | 1.480773 |

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|---|---|---|---|---|---|---|
| 147 | 5 | 1 | 1.493024 | 1.481661 | 1.487639 | 1.478839 |
| 148 | 5 | | 1.493128 | 1.482229 | 1.491059 | 1.482228 |
| 149 | 4 | | 1.492060 | 1.484109 | 1.492961 | 1.484109 |
| 150 | 4 | | 1.492458 | 1.479626 | 1.484683 | 1.475935 |
| 151 | 4 | | 1.491943 | 1.477271 | 1.452740 | 1.444214 |
| 152 | 5 | | 1.491892 | 1.477952 | 1.486688 | 1.477952 |
| 153 | 3 | | 1.491808 | 1.476801 | 1.485513 | 1.476801 |
| 154 | 4 | | 1.490120 | 1.478195 | 1.486939 | 1.478195 |
| 155 | 5 | | 1.494134 | 1.478340 | 1.487088 | 1.478340 |
| 156 | 6 | 1 | 1.495917 | 1.483243 | 1.492096 | 1.483243 |
| 157 | 5 | | 1.493647 | 1.485315 | 1.494206 | 1.485315 |
| 158 | 5 | | 1.492941 | 1.478347 | 1.487099 | 1.478347 |
| 159 | 5 | | 1.490737 | 1.482753 | 1.491593 | 1.482753 |
| 160 | 4 | | 1.490263 | 1.482190 | 1.491013 | 1.482190 |
| 161 | 4 | | 1.493646 | 1.479083 | 1.487842 | 1.479083 |
| 162 | 6 | 1 | 1.495802 | 1.483155 | 1.489466 | 1.480638 |
| 163 | 5 | | 1.495283 | 1.480911 | 1.489714 | 1.480911 |
| 164 | 6 | | 1.493410 | 1.489267 | 1.498233 | 1.489267 |
| 165 | 5 | | 1.493151 | 1.478785 | 1.487541 | 1.478785 |
| 166 | 6 | | 1.493894 | 1.483036 | 1.491876 | 1.483036 |
| 167 | 5 | 3 | 1.493500 | 1.485819 | 1.483702 | 1.474864 |
| 168 | 6 | 1 | 1.495272 | 1.481693 | 1.490505 | 1.481693 |
| 169 | 5 | | 1.493002 | 1.478274 | 1.487017 | 1.478273 |
| 170 | 6 | 1 | 1.494384 | 1.483056 | 1.479295 | 1.470534 |
| 171 | 6 | | 1.492940 | 1.481199 | 1.490005 | 1.481199 |
| 172 | 5 | | 1.493382 | 1.480257 | 1.489044 | 1.480257 |
| 173 | 5 | 2 | 1.494473 | 1.472474 | 1.481098 | 1.472474 |
| 174 | 4 | | 1.493911 | 1.477187 | 1.485907 | 1.477187 |
| 175 | 4 | | 1.496340 | 1.477490 | 1.486158 | 1.477436 |
| 176 | 4 | 1 | 1.496427 | 1.477120 | 1.485839 | 1.477120 |
| 177 | 5 | | 1.488345 | 1.484797 | 1.493680 | 1.484796 |
| 178 | 5 | | 1.494756 | 1.483607 | 1.492457 | 1.483607 |
| 179 | 3 | | 1.489547 | 1.487243 | 1.496172 | 1.487243 |
| 180 | 4 | | 1.495582 | 1.482864 | 1.491688 | 1.482851 |
| 181 | 3 | | 1.492722 | 1.485568 | 1.494453 | 1.485568 |
| 182 | 3 | | 1.495098 | 1.486703 | 1.495608 | 1.486703 |
| 183 | 4 | | 1.491496 | 1.487506 | 1.496424 | 1.487493 |
| 184 | 3 | | 1.493250 | 1.484575 | 1.493455 | 1.484575 |
| 185 | 6 | | 1.492920 | 1.483225 | 1.492077 | 1.483225 |
| 186 | 6 | | 1.490232 | 1.486766 | 1.495684 | 1.486766 |

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|---|---|---|---|---|---|
| 187 | 4 | 1.494128 | 1.482665 | 1.491491 | 1.482665 |
| 188 | 5 | 1.495308 | 1.482067 | 1.490886 | 1.482067 |
| 189 | 5 | 1.500157 | 1.480061 | 1.488840 | 1.480061 |
| 190 | 4 | 1.496487 | 1.481981 | 1.490806 | 1.481981 |
| 191 | 4 | 1.492405 | 1.477892 | 1.455883 | 1.447331 |
| 192 | 4 | 1.492786 | 1.481102 | 1.489904 | 1.481102 |
| 193 | 5 | 1.490073 | 1.480501 | 1.489294 | 1.480501 |
| 194 | 3 | 1.495864 | 1.479148 | 1.487901 | 1.479148 |
| 195 | 3 | 1.491782 | 1.483725 | 1.492588 | 1.483725 |
| 196 | 3 | 1.496284 | 1.482415 | 1.491244 | 1.482415 |
| 197 | 4 | 1.493084 | 1.475771 | 1.484455 | 1.475771 |
| 198 | 5 | 1.491601 | 1.478331 | 1.487070 | 1.478331 |
| 199 | 5 | 1.491311 | 1.478918 | 1.469607 | 1.460958 |
| 200 | 4 | 1.491066 | 1.476528 | 1.485230 | 1.476528 |

## lg-$^{37}$Cl/$^{35}$Cl isotopic partition-function ratios for (NC$^{-}$···EtCl).*n*DMSO reactant structures:

| structure sequence number | *n* | number extra imaginaries | extra imaginaries treated as reals | | extra imaginaries omitted | |
|---|---|---|---|---|---|---|
| | | | 300 K | 303.15K | 300 K | 303.15K |
| | | | $f_{RS}$ | $f_{RS}$ | $f_{RS}$ | $f_{RS}$ |
| 1 | 4 | | 1.009940 | 1.010489 | 1.010679 | 1.010489 |
| 2 | 5 | 1 | 1.010239 | 1.009905 | 0.993815 | 0.993638 |
| 3 | 4 | | 1.010248 | 1.010177 | 1.010362 | 1.010177 |
| 4 | 4 | | 1.010497 | 1.010219 | 1.010405 | 1.010219 |
| 5 | 4 | | 1.010332 | 1.010175 | 1.010359 | 1.010175 |
| 6 | 7 | | 1.010430 | 1.010212 | 1.010397 | 1.010212 |
| 7 | 3 | | 1.010372 | 1.010134 | 1.010317 | 1.010134 |
| 8 | 6 | 1 | 1.010054 | 1.009993 | 1.010173 | 1.009991 |
| 9 | 5 | | 1.010359 | 1.010092 | 1.010274 | 1.010092 |
| 10 | 1 | 10 | 1.010354 | 1.010576 | 0.992161 | 0.991974 |
| 11 | 4 | 1 | 1.010167 | 1.010156 | 1.010239 | 1.010055 |
| 12 | 3 | | 1.010440 | 1.009743 | 1.009921 | 1.009743 |
| 13 | 4 | | 1.010005 | 1.010138 | 1.010322 | 1.010138 |
| 14 | 5 | | 1.010484 | 1.010459 | 1.010648 | 1.010459 |
| 15 | 5 | | 1.010207 | 1.010270 | 1.010456 | 1.010270 |
| 16 | 4 | 2 | 1.010135 | 1.010026 | 0.995741 | 0.995561 |
| 17 | 7 | 1 | 1.010043 | 1.010205 | 1.010278 | 1.010093 |
| 18 | 5 | | 1.010338 | 1.009927 | 1.010107 | 1.009927 |
| 19 | 3 | | 1.010548 | 1.010084 | 1.010267 | 1.010084 |
| 20 | 2 | | 1.010256 | 1.009763 | 1.009941 | 1.009763 |
| 21 | 3 | | 1.010300 | 1.010126 | 1.010309 | 1.010126 |
| 22 | 5 | | 1.010179 | 1.010066 | 1.010249 | 1.010067 |
| 23 | 2 | | 1.010521 | 1.010058 | 1.010241 | 1.010058 |
| 24 | 4 | | 1.010285 | 1.009882 | 1.010062 | 1.009882 |
| 25 | 3 | | 1.010491 | 1.010422 | 1.010611 | 1.010422 |
| 26 | 5 | | 1.010267 | 1.009951 | 1.010132 | 1.009951 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 27 | 6 | | 1.010131 | 1.009789 | 1.009967 | 1.009789 |
| 28 | 5 | | 1.010178 | 1.010026 | 1.010208 | 1.010026 |
| 29 | 6 | | 1.010263 | 1.010122 | 1.010306 | 1.010122 |
| 30 | 5 | 1 | 1.010583 | 1.010121 | 0.992470 | 0.992290 |
| 31 | 4 | | 1.010065 | 1.010353 | 1.010540 | 1.010353 |
| 32 | 3 | | 1.009796 | 1.010108 | 1.010292 | 1.010108 |
| 33 | 2 | | 1.010225 | 1.010071 | 1.010253 | 1.010071 |
| 34 | 5 | | 1.010355 | 1.010158 | 1.010343 | 1.010158 |
| 35 | 6 | | 1.010245 | 1.010110 | 1.010293 | 1.010110 |
| 36 | 6 | | 1.010311 | 1.010128 | 1.010311 | 1.010128 |
| 37 | 5 | | 1.010338 | 1.010251 | 1.010437 | 1.010251 |
| 38 | 5 | | 1.010104 | 1.010073 | 1.010257 | 1.010073 |
| 39 | 4 | | 1.010151 | 1.010077 | 1.010260 | 1.010077 |
| 40 | 5 | 1 | 1.010223 | 1.010087 | 1.009333 | 1.009150 |
| 41 | 5 | | 1.009962 | 1.009891 | 1.010070 | 1.009891 |
| 42 | 4 | | 1.010173 | 1.009942 | 1.010124 | 1.009942 |
| 43 | 2 | | 1.010244 | 1.010061 | 1.010244 | 1.010061 |
| 44 | 6 | | 1.010284 | 1.010156 | 1.010340 | 1.010156 |
| 45 | 5 | 1 | 1.010183 | 1.009960 | 1.008875 | 1.008695 |
| 46 | 4 | | 1.010247 | 1.010144 | 1.010328 | 1.010144 |
| 47 | 4 | 1 | 1.010346 | 1.010090 | 1.010264 | 1.010081 |
| 48 | 3 | | 1.010323 | 1.010206 | 1.010391 | 1.010206 |
| 49 | 4 | | 1.010293 | 1.010114 | 1.010298 | 1.010114 |
| 50 | 4 | | 1.010075 | 1.010102 | 1.010286 | 1.010102 |
| 51 | 4 | | 1.009961 | 1.010162 | 1.010347 | 1.010162 |
| 52 | 3 | | 1.010049 | 1.010118 | 1.010302 | 1.010118 |
| 53 | 4 | | 1.009961 | 1.010131 | 1.010315 | 1.010131 |
| 54 | 4 | 1 | 1.010149 | 1.009925 | 1.010023 | 1.009843 |
| 55 | 2 | | 1.010122 | 1.010105 | 1.010288 | 1.010105 |
| 56 | 3 | | 1.010287 | 1.010291 | 1.010477 | 1.010291 |
| 57 | 2 | | 1.010448 | 1.010160 | 1.010344 | 1.010160 |
| 58 | 6 | | 1.010396 | 1.010136 | 1.010320 | 1.010136 |
| 59 | 2 | | 1.010332 | 1.010031 | 1.010213 | 1.010031 |
| 60 | 2 | | 1.010398 | 1.009953 | 1.010134 | 1.009953 |
| 61 | 4 | | 1.010122 | 1.010185 | 1.010370 | 1.010185 |
| 62 | 6 | | 1.010270 | 1.010432 | 1.010620 | 1.010432 |
| 63 | 4 | 1 | 1.010128 | 1.010303 | 0.996683 | 0.996499 |
| 64 | 4 | | 1.010678 | 1.010206 | 1.010391 | 1.010206 |
| 65 | 2 | | 1.010118 | 1.010044 | 1.010226 | 1.010044 |
| 66 | 4 | | 1.010308 | 1.010252 | 1.010438 | 1.010252 |

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|---|---|---|---|---|---|---|
| 67 | 3 | | 1.010373 | 1.010174 | 1.010359 | 1.010174 |
| 68 | 6 | | 1.010159 | 1.010272 | 1.010458 | 1.010272 |
| 69 | 5 | | 1.010050 | 1.010223 | 1.010409 | 1.010223 |
| 70 | 7 | 1 | 1.010250 | 1.010239 | 1.010424 | 1.010239 |
| 71 | 3 | | 1.010232 | 1.010138 | 1.010322 | 1.010138 |
| 72 | 5 | | 1.010247 | 1.010162 | 1.010346 | 1.010162 |
| 73 | 5 | | 1.009801 | 1.010209 | 1.010394 | 1.010209 |
| 74 | 3 | | 1.009923 | 1.010149 | 1.010333 | 1.010149 |
| 75 | 4 | | 1.010064 | 1.010474 | 1.010664 | 1.010474 |
| 76 | 4 | 1 | 1.010043 | 1.010398 | 1.010585 | 1.010397 |
| 77 | 6 | | 1.010510 | 1.009955 | 1.010136 | 1.009955 |
| 78 | 2 | | 1.010295 | 1.010218 | 1.010403 | 1.010218 |
| 79 | 5 | | 1.010583 | 1.010039 | 1.010221 | 1.010038 |
| 80 | 5 | | 1.010274 | 1.010290 | 1.010476 | 1.010290 |
| 81 | 3 | 1 | 1.010832 | 1.010288 | 1.007120 | 1.006934 |
| 82 | 4 | | 1.010631 | 1.010451 | 1.010641 | 1.010451 |
| 83 | 0 | | 1.010646 | 1.010112 | 1.010296 | 1.010112 |
| 84 | 4 | | 1.010376 | 1.010239 | 1.010425 | 1.010239 |
| 85 | 5 | | 1.010265 | 1.010205 | 1.010390 | 1.010205 |
| 86 | 7 | 2 | 1.010467 | 1.009980 | 1.007946 | 1.007765 |
| 87 | 6 | | 1.010276 | 1.010218 | 1.010403 | 1.010218 |
| 88 | 2 | | 1.010200 | 1.010445 | 1.010634 | 1.010445 |
| 89 | 5 | | 1.010162 | 1.010561 | 1.010752 | 1.010561 |
| 90 | 2 | | 1.010224 | 1.010403 | 1.010591 | 1.010403 |
| 91 | 4 | | 1.010018 | 1.010140 | 1.010324 | 1.010140 |
| 92 | 3 | | 1.010119 | 1.010053 | 1.010235 | 1.010053 |
| 93 | 6 | | 1.010178 | 1.010141 | 1.010325 | 1.010141 |
| 94 | 1 | | 1.010175 | 1.010374 | 1.010562 | 1.010374 |
| 95 | 2 | | 1.010377 | 1.010091 | 1.010275 | 1.010091 |
| 96 | 4 | | 1.010325 | 1.010445 | 1.010633 | 1.010445 |
| 97 | 3 | | 1.009832 | 1.010265 | 1.010451 | 1.010265 |
| 98 | 4 | | 1.010180 | 1.010121 | 1.010305 | 1.010121 |
| 99 | 4 | | 1.010148 | 1.010028 | 1.010210 | 1.010028 |
| 100 | 4 | | 1.010144 | 1.010175 | 1.010361 | 1.010175 |
| 101 | 3 | | 1.010679 | 1.009761 | 1.009677 | 1.009499 |
| 102 | 5 | | 1.010085 | 1.010055 | 1.010239 | 1.010055 |
| 103 | 5 | | 1.010362 | 1.010065 | 1.010248 | 1.010065 |
| 104 | 4 | | 1.010405 | 1.010310 | 1.010497 | 1.010310 |
| 105 | 5 | | 1.010359 | 1.010147 | 1.010332 | 1.010147 |
| 106 | 4 | | 1.010397 | 1.010244 | 1.010430 | 1.010244 |

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|---|---|---|---|---|---|---|
| 107 | 5 | 3 | 1.010317 | 1.010188 | 1.010372 | 1.010188 |
| 108 | 4 | 2 | 1.010175 | 1.009875 | 1.010055 | 1.009875 |
| 109 | 3 | 1 | 1.010274 | 1.010174 | 1.010359 | 1.010174 |
| 110 | 4 | | 1.010766 | 1.010169 | 1.009195 | 1.009010 |
| 111 | 3 | | 1.010340 | 1.009985 | 1.010167 | 1.009985 |
| 112 | 4 | | 1.009921 | 1.010253 | 1.010440 | 1.010253 |
| 113 | 3 | | 1.010322 | 1.009825 | 1.010005 | 1.009825 |
| 114 | 3 | | 1.010648 | 1.010296 | 1.010484 | 1.010296 |
| 115 | 4 | | 1.010456 | 1.010024 | 1.010207 | 1.010024 |
| 116 | 4 | | 1.010208 | 1.009953 | 1.010135 | 1.009953 |
| 117 | 4 | | 1.010390 | 1.009863 | 1.010043 | 1.009863 |
| 118 | 4 | | 1.010107 | 1.010153 | 1.010338 | 1.010153 |
| 119 | 3 | 19 | 1.010267 | 1.010360 | 1.010548 | 1.010360 |
| 120 | 4 | | 1.009941 | 1.010073 | 1.010256 | 1.010073 |
| 121 | 4 | | 1.010309 | 1.010116 | 1.010300 | 1.010116 |
| 122 | 3 | 1 | 1.010249 | 1.009997 | 1.010179 | 1.009997 |
| 123 | 5 | 1 | 1.010241 | 1.010334 | 1.010521 | 1.010334 |
| 124 | 5 | 1 | 1.010062 | 1.010101 | 1.010210 | 1.010026 |
| 125 | 4 | | 1.010611 | 1.010304 | 1.010491 | 1.010304 |
| 126 | 4 | | 1.010132 | 1.010083 | 1.010267 | 1.010083 |
| 127 | 5 | 1 | 1.009967 | 1.009949 | 1.010131 | 1.009949 |
| 128 | 4 | | 1.010208 | 1.009996 | 1.010178 | 1.009996 |
| 129 | 4 | | 1.010306 | 1.010080 | 1.010263 | 1.010080 |
| 130 | 4 | 1 | 1.010305 | 1.010393 | 1.010583 | 1.010393 |
| 131 | 5 | | 1.010540 | 1.009884 | 1.010064 | 1.009884 |
| 132 | 5 | 1 | 1.010292 | 1.009619 | 1.009796 | 1.009620 |
| 133 | 4 | 2 | 1.010253 | 1.010042 | 1.010225 | 1.010042 |
| 134 | 4 | | 1.010343 | 1.010170 | 1.010355 | 1.010170 |
| 135 | 3 | | 1.010293 | 1.010062 | 1.010245 | 1.010062 |
| 136 | 4 | 1 | 1.010311 | 1.010127 | 1.010311 | 1.010127 |
| 137 | 2 | | 1.010437 | 1.010154 | 0.990331 | 0.990150 |
| 138 | 4 | 2 | 1.010257 | 1.009923 | 1.010104 | 1.009923 |
| 139 | 3 | | 1.010260 | 1.009969 | 1.010151 | 1.009969 |
| 140 | 3 | | 1.010270 | 1.010039 | 1.010223 | 1.010039 |
| 141 | 5 | | 1.010070 | 1.009783 | 1.009962 | 1.009783 |
| 142 | 4 | | 1.010124 | 1.009991 | 1.010173 | 1.009991 |
| 143 | 5 | | 1.010244 | 1.010060 | 1.010244 | 1.010060 |
| 144 | 4 | | 1.010340 | 1.010100 | 1.010284 | 1.010100 |
| 145 | 5 | | 1.010141 | 1.010001 | 1.010183 | 1.010001 |
| 146 | 5 | | 1.010328 | 1.010063 | 1.010247 | 1.010063 |

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|---|---|---|---|---|---|---|
| 147 | 5 | 1 | 1.010273 | 1.010160 | 1.008681 | 1.008496 |
| 148 | 5 | | 1.010391 | 1.010138 | 1.010323 | 1.010138 |
| 149 | 4 | | 1.010298 | 1.010110 | 1.010293 | 1.010110 |
| 150 | 4 | | 1.010286 | 1.009894 | 1.007132 | 1.006952 |
| 151 | 4 | | 1.010347 | 1.009782 | 1.005347 | 1.005169 |
| 152 | 5 | | 1.010302 | 1.009869 | 1.010049 | 1.009869 |
| 153 | 3 | | 1.010315 | 1.009782 | 1.009961 | 1.009782 |
| 154 | 4 | | 1.010106 | 1.009967 | 1.010149 | 1.009967 |
| 155 | 5 | | 1.010288 | 1.009940 | 1.010122 | 1.009940 |
| 156 | 6 | 1 | 1.010477 | 1.010103 | 1.010287 | 1.010103 |
| 157 | 5 | | 1.010344 | 1.010262 | 1.010448 | 1.010262 |
| 158 | 5 | | 1.010320 | 1.010209 | 1.010396 | 1.010209 |
| 159 | 5 | | 1.010213 | 1.010148 | 1.010332 | 1.010148 |
| 160 | 4 | | 1.010134 | 1.010212 | 1.010398 | 1.010212 |
| 161 | 4 | | 1.010370 | 1.009941 | 1.010122 | 1.009941 |
| 162 | 6 | 1 | 1.010620 | 1.010086 | 1.009265 | 1.009082 |
| 163 | 5 | | 1.010490 | 1.009947 | 1.010128 | 1.009947 |
| 164 | 6 | | 1.010391 | 1.010489 | 1.010678 | 1.010489 |
| 165 | 5 | | 1.010226 | 1.009936 | 1.010118 | 1.009936 |
| 166 | 6 | | 1.010438 | 1.010124 | 1.010308 | 1.010124 |
| 167 | 5 | 3 | 1.010359 | 1.010189 | 1.002584 | 1.002401 |
| 168 | 6 | 1 | 1.010458 | 1.009978 | 1.010159 | 1.009978 |
| 169 | 5 | | 1.010409 | 1.009870 | 1.010050 | 1.009870 |
| 170 | 6 | 1 | 1.010424 | 1.010067 | 0.989550 | 0.989371 |
| 171 | 6 | | 1.010322 | 1.010049 | 1.010232 | 1.010049 |
| 172 | 5 | | 1.010346 | 1.010063 | 1.010247 | 1.010063 |
| 173 | 5 | 2 | 1.010394 | 1.009624 | 1.009801 | 1.009624 |
| 174 | 4 | | 1.010333 | 1.009745 | 1.009923 | 1.009745 |
| 175 | 4 | | 1.010664 | 1.009884 | 1.010027 | 1.009846 |
| 176 | 4 | 1 | 1.010585 | 1.009863 | 1.010043 | 1.009863 |
| 177 | 5 | | 1.010136 | 1.010323 | 1.010510 | 1.010322 |
| 178 | 5 | | 1.010403 | 1.010111 | 1.010295 | 1.010111 |
| 179 | 3 | | 1.010221 | 1.010395 | 1.010583 | 1.010395 |
| 180 | 4 | | 1.010476 | 1.010090 | 1.010254 | 1.010071 |
| 181 | 3 | | 1.010475 | 1.010639 | 1.010832 | 1.010639 |
| 182 | 3 | | 1.010641 | 1.010442 | 1.010632 | 1.010443 |
| 183 | 4 | | 1.010296 | 1.010457 | 1.010638 | 1.010449 |
| 184 | 3 | | 1.010425 | 1.010191 | 1.010377 | 1.010192 |
| 185 | 6 | | 1.010390 | 1.010082 | 1.010265 | 1.010082 |
| 186 | 6 | | 1.010161 | 1.010281 | 1.010467 | 1.010281 |

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|---|---|---|---|---|---|
| 187 | 4 | 1.010403 | 1.010093 | 1.010276 | 1.010093 |
| 188 | 5 | 1.010634 | 1.010018 | 1.010200 | 1.010018 |
| 189 | 5 | 1.010752 | 1.009980 | 1.010162 | 1.009980 |
| 190 | 4 | 1.010591 | 1.010041 | 1.010224 | 1.010041 |
| 191 | 4 | 1.010324 | 1.009839 | 1.004395 | 1.004216 |
| 192 | 4 | 1.010235 | 1.009938 | 1.010119 | 1.009938 |
| 193 | 5 | 1.010325 | 1.009996 | 1.010178 | 1.009996 |
| 194 | 3 | 1.010562 | 1.009993 | 1.010175 | 1.009993 |
| 195 | 3 | 1.010275 | 1.010192 | 1.010377 | 1.010192 |
| 196 | 3 | 1.010633 | 1.010140 | 1.010325 | 1.010140 |
| 197 | 4 | 1.010451 | 1.009656 | 1.009832 | 1.009656 |
| 198 | 5 | 1.010305 | 1.009997 | 1.010180 | 1.009997 |
| 199 | 5 | 1.010210 | 1.009966 | 0.992390 | 0.992211 |
| 200 | 4 | 1.010361 | 1.009962 | 1.010144 | 1.009962 |

## nu-$^{13}C/^{12}C$ isotopic partition-function ratios for ($NC^{-}\cdots EtCl$).*n*DMSO reactant structures:

| structure sequence number | *n* | number extra imaginaries | abnormal* | extra imaginaries treated as reals | | extra imaginaries omitted | |
|---|---|---|---|---|---|---|---|
| | | | | 300 K | 303.15K | 300 K | 303.15K |
| | | | | $f_{RS}$ | $f_{RS}$ | $f_{RS}$ | $f_{RS}$ |
| 1 | 4 | | * | 1.116211 | 1.108452 | 1.109943 | 1.108452 |
| 2 | 5 | 1 | | 1.113856 | 1.111586 | 1.113122 | 1.111580 |
| 3 | 4 | | | 1.108669 | 1.124971 | 1.126748 | 1.124971 |
| 4 | 4 | | | 1.115215 | 1.111433 | 1.112969 | 1.111433 |
| 5 | 4 | | | 1.130445 | 1.120358 | 1.122059 | 1.120358 |
| 6 | 7 | | * | 1.113486 | 1.128289 | 1.130154 | 1.128289 |
| 7 | 3 | | * | 1.129724 | 1.125587 | 1.127400 | 1.125587 |
| 8 | 6 | 1 | * | 1.129036 | 1.128212 | 1.129884 | 1.128023 |
| 9 | 5 | | | 1.130447 | 1.129439 | 1.131281 | 1.129439 |
| 10 | 1 | 10 | * | 1.133034 | 1.106147 | 1.063134 | 1.061776 |
| 11 | 4 | 1 | * | 1.115967 | 1.127141 | 1.128935 | 1.127093 |
| 12 | 3 | | | 1.130821 | 1.140291 | 1.142282 | 1.140291 |
| 13 | 4 | | | 1.109380 | 1.131190 | 1.133060 | 1.131191 |
| 14 | 5 | | | 1.131310 | 1.123103 | 1.124842 | 1.123103 |
| 15 | 5 | | | 1.108749 | 1.114023 | 1.115605 | 1.114023 |
| 16 | 4 | 2 | | 1.129358 | 1.120514 | 1.121269 | 1.119575 |
| 17 | 7 | 1 | | 1.107933 | 1.113304 | 1.114679 | 1.113110 |
| 18 | 5 | | | 1.110336 | 1.112904 | 1.114470 | 1.112904 |
| 19 | 3 | | | 1.119492 | 1.111840 | 1.113390 | 1.111840 |
| 20 | 2 | | * | 1.114799 | 1.127867 | 1.129722 | 1.127867 |
| 21 | 3 | | * | 1.112945 | 1.127829 | 1.129681 | 1.127829 |
| 22 | 5 | | | 1.130361 | 1.113769 | 1.115350 | 1.113769 |
| 23 | 2 | | | 1.111475 | 1.119567 | 1.121247 | 1.119567 |
| 24 | 4 | | | 1.112133 | 1.111045 | 1.112576 | 1.111045 |
| 25 | 3 | | | 1.116282 | 1.135570 | 1.137505 | 1.135570 |
| 26 | 5 | | | 1.113837 | 1.122398 | 1.124126 | 1.122398 |

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|---|---|---|---|---|---|---|---|
| 27 | 6 | | * | 1.130093 | 1.125155 | 1.126959 | 1.125154 |
| 28 | 5 | | | 1.128861 | 1.123103 | 1.124848 | 1.123103 |
| 29 | 6 | | * | 1.114196 | 1.106218 | 1.107669 | 1.106218 |
| 30 | 5 | 1 | * | 1.134180 | 1.130240 | 1.132139 | 1.130240 |
| 31 | 4 | | | 1.121428 | 1.121272 | 1.122980 | 1.121272 |
| 32 | 3 | | | 1.122678 | 1.146538 | 1.148624 | 1.146538 |
| 33 | 2 | | | 1.129805 | 1.146066 | 1.148143 | 1.146066 |
| 34 | 5 | | | 1.128835 | 1.126437 | 1.128238 | 1.126437 |
| 35 | 6 | | | 1.130105 | 1.145140 | 1.147199 | 1.145140 |
| 36 | 6 | | | 1.119553 | 1.125163 | 1.126939 | 1.125163 |
| 37 | 5 | | | 1.121577 | 1.120499 | 1.122196 | 1.120499 |
| 38 | 5 | | | 1.119493 | 1.113662 | 1.115241 | 1.113662 |
| 39 | 4 | | | 1.114622 | 1.112634 | 1.114191 | 1.112634 |
| 40 | 5 | 1 | | 1.122978 | 1.115505 | 1.117108 | 1.115500 |
| 41 | 5 | | * | 1.127337 | 1.106442 | 1.107895 | 1.106442 |
| 42 | 4 | | | 1.108894 | 1.119982 | 1.121672 | 1.119982 |
| 43 | 2 | | | 1.115849 | 1.114401 | 1.115994 | 1.114401 |
| 44 | 6 | | | 1.111275 | 1.116282 | 1.117907 | 1.116282 |
| 45 | 5 | 1 | | 1.108727 | 1.114172 | 1.115627 | 1.114037 |
| 46 | 4 | | | 1.112629 | 1.138309 | 1.140300 | 1.138309 |
| 47 | 4 | 1 | * | 1.128361 | 1.128455 | 1.130317 | 1.128455 |
| 48 | 3 | | | 1.117815 | 1.119833 | 1.121524 | 1.119833 |
| 49 | 4 | | | 1.111833 | 1.119121 | 1.120792 | 1.119121 |
| 50 | 4 | | | 1.117132 | 1.110396 | 1.111914 | 1.110396 |
| 51 | 4 | | | 1.117761 | 1.110258 | 1.111780 | 1.110258 |
| 52 | 3 | | | 1.117571 | 1.119878 | 1.121566 | 1.119878 |
| 53 | 4 | | * | 1.120411 | 1.106481 | 1.107938 | 1.106481 |
| 54 | 4 | 1 | * | 1.116650 | 1.108324 | 1.086050 | 1.084588 |
| 55 | 2 | | | 1.111874 | 1.125448 | 1.127228 | 1.125448 |
| 56 | 3 | | * | 1.117613 | 1.129762 | 1.131659 | 1.129762 |
| 57 | 2 | | | 1.111412 | 1.105165 | 1.106596 | 1.105165 |
| 58 | 6 | | * | 1.113813 | 1.107031 | 1.108495 | 1.107031 |
| 59 | 2 | | | 1.118639 | 1.108561 | 1.110055 | 1.108561 |
| 60 | 2 | | | 1.115963 | 1.120985 | 1.122692 | 1.120985 |
| 61 | 4 | | * | 1.131041 | 1.126689 | 1.128521 | 1.126689 |
| 62 | 6 | | * | 1.111877 | 1.126296 | 1.128120 | 1.126296 |
| 63 | 4 | 1 | * | 1.129380 | 1.114788 | 1.116386 | 1.114787 |
| 64 | 4 | | | 1.114724 | 1.113188 | 1.114762 | 1.113188 |
| 65 | 2 | | | 1.107363 | 1.114809 | 1.116412 | 1.114809 |
| 66 | 4 | | | 1.108915 | 1.114628 | 1.116223 | 1.114628 |

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|---|---|---|---|---|---|---|---|
| 67 | 3 | | | 1.126427 | 1.120010 | 1.121704 | 1.120010 |
| 68 | 6 | | | 1.114340 | 1.117774 | 1.119425 | 1.117774 |
| 69 | 5 | | | 1.107839 | 1.117841 | 1.119495 | 1.117841 |
| 70 | 7 | 1 | | 1.128108 | 1.113457 | 1.114355 | 1.112782 |
| 71 | 3 | | | 1.128425 | 1.104806 | 1.106223 | 1.104806 |
| 72 | 5 | | * | 1.107890 | 1.106462 | 1.107910 | 1.106462 |
| 73 | 5 | | | 1.128030 | 1.109874 | 1.111386 | 1.109874 |
| 74 | 3 | | | 1.108983 | 1.113837 | 1.115417 | 1.113837 |
| 75 | 4 | | | 1.119640 | 1.115200 | 1.116807 | 1.115200 |
| 76 | 4 | 1 | | 1.118810 | 1.113399 | 1.113906 | 1.112335 |
| 77 | 6 | | | 1.108753 | 1.116049 | 1.117670 | 1.116049 |
| 78 | 2 | | * | 1.112837 | 1.105645 | 1.107109 | 1.105645 |
| 79 | 5 | | | 1.129730 | 1.118896 | 1.120564 | 1.118896 |
| 80 | 5 | | * | 1.109561 | 1.128203 | 1.130065 | 1.128203 |
| 81 | 3 | 1 | * | 1.109306 | 1.126439 | 1.128274 | 1.126439 |
| 82 | 4 | | | 1.108374 | 1.135178 | 1.137108 | 1.135178 |
| 83 | 0 | | | 1.128713 | 1.107028 | 1.108495 | 1.107028 |
| 84 | 4 | | | 1.107575 | 1.120465 | 1.122160 | 1.120465 |
| 85 | 5 | | * | 1.107195 | 1.127320 | 1.129168 | 1.127320 |
| 86 | 7 | 2 | * | 1.130546 | 1.127245 | 1.128276 | 1.126435 |
| 87 | 6 | | | 1.137668 | 1.126181 | 1.127980 | 1.126181 |
| 88 | 2 | | | 1.115768 | 1.119641 | 1.121325 | 1.119641 |
| 89 | 5 | | * | 1.117107 | 1.107095 | 1.108562 | 1.107095 |
| 90 | 2 | | | 1.108323 | 1.113213 | 1.114784 | 1.113213 |
| 91 | 4 | | * | 1.116061 | 1.127110 | 1.128951 | 1.127110 |
| 92 | 3 | | * | 1.111087 | 1.125285 | 1.127090 | 1.125285 |
| 93 | 6 | | * | 1.128311 | 1.125474 | 1.127284 | 1.125474 |
| 94 | 1 | | | 1.120032 | 1.106207 | 1.107654 | 1.106207 |
| 95 | 2 | | | 1.120853 | 1.115628 | 1.117244 | 1.115628 |
| 96 | 4 | | * | 1.129214 | 1.107922 | 1.109430 | 1.107922 |
| 97 | 3 | | | 1.130960 | 1.110787 | 1.112314 | 1.110787 |
| 98 | 4 | | | 1.129313 | 1.121171 | 1.122882 | 1.121171 |
| 99 | 4 | | | 1.114873 | 1.112832 | 1.114402 | 1.112832 |
| 100 | 4 | | | 1.126861 | 1.115869 | 1.117487 | 1.115869 |
| 101 | 3 | | | 1.109944 | 1.114619 | 1.116211 | 1.114619 |
| 102 | 5 | | | 1.113128 | 1.112300 | 1.113856 | 1.112300 |
| 103 | 5 | | * | 1.126748 | 1.107201 | 1.108669 | 1.107201 |
| 104 | 4 | | | 1.112969 | 1.113635 | 1.115215 | 1.113635 |
| 105 | 5 | | * | 1.122059 | 1.128577 | 1.130445 | 1.128577 |
| 106 | 4 | | | 1.130154 | 1.111937 | 1.113486 | 1.111937 |

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|---|---|---|---|---|---|---|---|
| 107 | 5 | 3 | * | 1.127400 | 1.127869 | 1.129397 | 1.127542 |
| 108 | 4 | 2 | * | 1.130074 | 1.127192 | 1.128191 | 1.126348 |
| 109 | 3 | 1 | * | 1.131281 | 1.128578 | 1.128075 | 1.126210 |
| 110 | 4 | | | 1.107586 | 1.131163 | 1.133034 | 1.131163 |
| 111 | 3 | | | 1.128983 | 1.114373 | 1.115967 | 1.114373 |
| 112 | 4 | | * | 1.142282 | 1.128945 | 1.130821 | 1.128945 |
| 113 | 3 | | * | 1.133060 | 1.107899 | 1.109380 | 1.107899 |
| 114 | 3 | | * | 1.124842 | 1.129428 | 1.131310 | 1.129428 |
| 115 | 4 | | * | 1.115605 | 1.107283 | 1.108749 | 1.107283 |
| 116 | 4 | | * | 1.122209 | 1.127511 | 1.129358 | 1.127511 |
| 117 | 4 | | * | 1.114873 | 1.106484 | 1.107933 | 1.106485 |
| 118 | 4 | | * | 1.114470 | 1.108847 | 1.110336 | 1.108847 |
| 119 | 3 | 19 | * | 1.113390 | 1.117847 | 1.054456 | 1.053068 |
| 120 | 4 | | | 1.129722 | 1.113230 | 1.114799 | 1.113230 |
| 121 | 4 | | | 1.129681 | 1.111409 | 1.112945 | 1.111409 |
| 122 | 3 | 1 | * | 1.115350 | 1.128496 | 1.130003 | 1.128138 |
| 123 | 5 | 1 | * | 1.121247 | 1.109960 | 1.109625 | 1.108113 |
| 124 | 5 | 1 | | 1.112576 | 1.110597 | 1.107405 | 1.105875 |
| 125 | 4 | | | 1.137505 | 1.114686 | 1.116282 | 1.114686 |
| 126 | 4 | | | 1.124126 | 1.112283 | 1.113837 | 1.112283 |
| 127 | 5 | 1 | * | 1.126961 | 1.128233 | 1.127778 | 1.125921 |
| 128 | 4 | | * | 1.124848 | 1.127021 | 1.128861 | 1.127021 |
| 129 | 4 | | | 1.107669 | 1.112635 | 1.114196 | 1.112635 |
| 130 | 4 | 1 | | 1.132139 | 1.132283 | 1.131413 | 1.129521 |
| 131 | 5 | | | 1.122980 | 1.119748 | 1.121429 | 1.119749 |
| 132 | 5 | 1 | | 1.148624 | 1.120969 | 1.120048 | 1.118343 |
| 133 | 4 | 2 | * | 1.148143 | 1.127948 | 1.124944 | 1.123095 |
| 134 | 4 | | * | 1.128238 | 1.126995 | 1.128835 | 1.126995 |
| 135 | 3 | | * | 1.147199 | 1.128243 | 1.130105 | 1.128243 |
| 136 | 4 | 1 | | 1.126939 | 1.117898 | 1.117328 | 1.115676 |
| 137 | 2 | | | 1.122196 | 1.119889 | 1.121577 | 1.119889 |
| 138 | 4 | 2 | | 1.115241 | 1.117841 | 1.119177 | 1.117526 |
| 139 | 3 | | | 1.114191 | 1.113055 | 1.114622 | 1.113055 |
| 140 | 3 | | | 1.117113 | 1.121265 | 1.122978 | 1.121265 |
| 141 | 5 | | | 1.107895 | 1.125550 | 1.127337 | 1.125550 |
| 142 | 4 | | * | 1.121672 | 1.107422 | 1.108894 | 1.107422 |
| 143 | 5 | | | 1.115994 | 1.114262 | 1.115849 | 1.114262 |
| 144 | 4 | | | 1.117907 | 1.109765 | 1.111275 | 1.109765 |
| 145 | 5 | | * | 1.115761 | 1.107262 | 1.108727 | 1.107262 |
| 146 | 5 | | | 1.140300 | 1.111096 | 1.112629 | 1.111097 |

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|---|---|---|---|---|---|---|---|
| 147 | 5 | 1 | * | 1.130317 | 1.126532 | 1.127444 | 1.125617 |
| 148 | 5 | | | 1.121524 | 1.116191 | 1.117815 | 1.116191 |
| 149 | 4 | | | 1.120792 | 1.110314 | 1.111833 | 1.110314 |
| 150 | 4 | | | 1.111914 | 1.115522 | 1.117132 | 1.115522 |
| 151 | 4 | | | 1.111780 | 1.116144 | 1.117761 | 1.116144 |
| 152 | 5 | | | 1.121566 | 1.115951 | 1.117571 | 1.115951 |
| 153 | 3 | | | 1.107938 | 1.118746 | 1.120411 | 1.118746 |
| 154 | 4 | | | 1.109820 | 1.115043 | 1.116650 | 1.115043 |
| 155 | 5 | | | 1.127229 | 1.110356 | 1.111874 | 1.110356 |
| 156 | 6 | 1 | | 1.131659 | 1.115994 | 1.117607 | 1.115988 |
| 157 | 5 | | | 1.106596 | 1.109899 | 1.111412 | 1.109899 |
| 158 | 5 | | | 1.108495 | 1.112257 | 1.113813 | 1.112257 |
| 159 | 5 | | | 1.110055 | 1.117003 | 1.118639 | 1.117003 |
| 160 | 4 | | | 1.122692 | 1.114369 | 1.115963 | 1.114369 |
| 161 | 4 | | * | 1.128521 | 1.129164 | 1.131041 | 1.129164 |
| 162 | 6 | 1 | | 1.128120 | 1.110355 | 1.107448 | 1.105933 |
| 163 | 5 | | * | 1.116388 | 1.127532 | 1.129380 | 1.127532 |
| 164 | 6 | | | 1.114762 | 1.113156 | 1.114724 | 1.113156 |
| 165 | 5 | | | 1.116412 | 1.105921 | 1.107363 | 1.105921 |
| 166 | 6 | | * | 1.116223 | 1.107445 | 1.108915 | 1.107445 |
| 167 | 5 | 3 | * | 1.121704 | 1.124631 | 1.124045 | 1.122253 |
| 168 | 6 | 1 | * | 1.119425 | 1.112772 | 1.111742 | 1.110178 |
| 169 | 5 | | * | 1.119495 | 1.106379 | 1.107839 | 1.106379 |
| 170 | 6 | 1 | * | 1.115031 | 1.126283 | 1.127729 | 1.125905 |
| 171 | 6 | | * | 1.106223 | 1.126592 | 1.128425 | 1.126592 |
| 172 | 5 | | * | 1.107910 | 1.106439 | 1.107890 | 1.106439 |
| 173 | 5 | 2 | * | 1.111386 | 1.126203 | 1.123822 | 1.122002 |
| 174 | 4 | | * | 1.115417 | 1.107513 | 1.108983 | 1.107513 |
| 175 | 4 | | | 1.116807 | 1.117985 | 1.119640 | 1.117985 |
| 176 | 4 | 1 | | 1.114972 | 1.117171 | 1.114401 | 1.112768 |
| 177 | 5 | | * | 1.117670 | 1.107284 | 1.108753 | 1.107284 |
| 178 | 5 | | | 1.107109 | 1.111298 | 1.112837 | 1.111298 |
| 179 | 3 | | * | 1.120564 | 1.127873 | 1.129730 | 1.127873 |
| 180 | 4 | | * | 1.130065 | 1.108054 | 1.109561 | 1.108054 |
| 181 | 3 | | * | 1.128274 | 1.107799 | 1.109306 | 1.107799 |
| 182 | 3 | | * | 1.137108 | 1.106912 | 1.108374 | 1.106912 |
| 183 | 4 | | * | 1.108495 | 1.126874 | 1.128713 | 1.126874 |
| 184 | 3 | | * | 1.122160 | 1.106129 | 1.107575 | 1.106129 |
| 185 | 6 | | | 1.129168 | 1.105756 | 1.107195 | 1.105756 |
| 186 | 6 | | | 1.129087 | 1.128712 | 1.130546 | 1.128712 |

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|---|---|---|---|---|---|---|
| 187 | 4 | | 1.127980 | 1.135736 | 1.137668 | 1.135736 |
| 188 | 5 | | 1.121325 | 1.114184 | 1.115768 | 1.114184 |
| 189 | 5 | | 1.108562 | 1.115500 | 1.117107 | 1.115500 |
| 190 | 4 | * | 1.114784 | 1.106854 | 1.108323 | 1.106854 |
| 191 | 4 | | 1.128951 | 1.114468 | 1.116061 | 1.114468 |
| 192 | 4 | | 1.127090 | 1.109579 | 1.111087 | 1.109579 |
| 193 | 5 | * | 1.127284 | 1.126482 | 1.128311 | 1.126482 |
| 194 | 3 | | 1.107654 | 1.118375 | 1.120032 | 1.118375 |
| 195 | 3 | | 1.117244 | 1.119180 | 1.120853 | 1.119180 |
| 196 | 3 | * | 1.109430 | 1.127368 | 1.129214 | 1.127368 |
| 197 | 4 | * | 1.112314 | 1.129082 | 1.130960 | 1.129082 |
| 198 | 5 | * | 1.122882 | 1.127466 | 1.129313 | 1.127466 |
| 199 | 5 | | 1.114402 | 1.113300 | 1.114873 | 1.113300 |
| 200 | 4 | | 1.117487 | 1.125088 | 1.126862 | 1.125089 |

* structure omitted from ensemble of 122 RS configurations for isotopic substitution in cyanide anion

## nu-$^{15}$N/$^{14}$N isotopic partition-function ratios for (NC$^{-}$···EtCl).*n*DMSO reactant structures:

| structure sequence number | *n* | number extra imaginaries | abnormal* | extra imaginaries treated as reals | | extra imaginaries omitted | |
|---|---|---|---|---|---|---|---|
| | | | | 300 K | 303.15K | 300 K | 303.15K |
| | | | | $f_{RS}$ | $f_{RS}$ | $f_{RS}$ | $f_{RS}$ |
| 1 | 4 | | * | 1.078916 | 1.076604 | 1.077630 | 1.076604 |
| 2 | 5 | 1 | | 1.078968 | 1.078029 | 1.079080 | 1.078025 |
| 3 | 4 | | | 1.078605 | 1.079064 | 1.080143 | 1.079064 |
| 4 | 4 | | | 1.079173 | 1.076945 | 1.077978 | 1.076945 |
| 5 | 4 | | | 1.083022 | 1.080407 | 1.081513 | 1.080407 |
| 6 | 7 | | * | 1.078717 | 1.081513 | 1.082640 | 1.081513 |
| 7 | 3 | | * | 1.082732 | 1.080556 | 1.081664 | 1.080556 |
| 8 | 6 | 1 | * | 1.082689 | 1.081216 | 1.080725 | 1.079606 |
| 9 | 5 | | | 1.083151 | 1.080580 | 1.081688 | 1.080580 |
| 10 | 1 | 10 | * | 1.082310 | 1.077139 | 1.039249 | 1.038273 |
| 11 | 4 | 1 | * | 1.078953 | 1.081388 | 1.082497 | 1.081371 |
| 12 | 3 | | | 1.082455 | 1.082171 | 1.083292 | 1.082171 |
| 13 | 4 | | | 1.078682 | 1.081163 | 1.082283 | 1.081164 |
| 14 | 5 | | | 1.082916 | 1.079418 | 1.080503 | 1.079418 |
| 15 | 5 | | | 1.078497 | 1.077309 | 1.078350 | 1.077309 |
| 16 | 4 | 2 | | 1.082900 | 1.078705 | 1.079311 | 1.078241 |
| 17 | 7 | 1 | | 1.078455 | 1.077605 | 1.078424 | 1.077376 |
| 18 | 5 | | | 1.077795 | 1.078025 | 1.079084 | 1.078025 |
| 19 | 3 | | | 1.086346 | 1.077676 | 1.078724 | 1.077676 |
| 20 | 2 | | * | 1.078386 | 1.081647 | 1.082778 | 1.081647 |
| 21 | 3 | | * | 1.078306 | 1.082123 | 1.083262 | 1.082123 |
| 22 | 5 | | | 1.082686 | 1.079027 | 1.080102 | 1.079027 |
| 23 | 2 | | | 1.078566 | 1.079052 | 1.080131 | 1.079052 |
| 24 | 4 | | | 1.078552 | 1.077057 | 1.078094 | 1.077057 |
| 25 | 3 | | | 1.078846 | 1.081710 | 1.082833 | 1.081710 |
| 26 | 5 | | | 1.078878 | 1.079729 | 1.080821 | 1.079729 |

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|---|---|---|---|---|---|---|---|
| 27 | 6 | | * | 1.082883 | 1.080318 | 1.081421 | 1.080317 |
| 28 | 5 | | | 1.082558 | 1.080074 | 1.081174 | 1.080074 |
| 29 | 6 | | * | 1.078761 | 1.076345 | 1.077371 | 1.076344 |
| 30 | 5 | 1 | * | 1.081919 | 1.081982 | 1.083118 | 1.081981 |
| 31 | 4 | | | 1.080174 | 1.079078 | 1.080156 | 1.079078 |
| 32 | 3 | | | 1.079941 | 1.083850 | 1.084994 | 1.083850 |
| 33 | 2 | | | 1.082265 | 1.083196 | 1.084326 | 1.083196 |
| 34 | 5 | | | 1.082276 | 1.080735 | 1.081849 | 1.080735 |
| 35 | 6 | | | 1.082965 | 1.083496 | 1.084632 | 1.083496 |
| 36 | 6 | | | 1.079877 | 1.079723 | 1.080815 | 1.079723 |
| 37 | 5 | | | 1.079345 | 1.078963 | 1.080038 | 1.078963 |
| 38 | 5 | | | 1.079628 | 1.077547 | 1.078593 | 1.077547 |
| 39 | 4 | | | 1.079944 | 1.078651 | 1.079721 | 1.078651 |
| 40 | 5 | 1 | | 1.080354 | 1.078434 | 1.079483 | 1.078419 |
| 41 | 5 | | * | 1.081081 | 1.077026 | 1.078062 | 1.077026 |
| 42 | 4 | | | 1.077840 | 1.078827 | 1.079899 | 1.078827 |
| 43 | 2 | | | 1.078757 | 1.078292 | 1.079351 | 1.078292 |
| 44 | 6 | | | 1.078233 | 1.078008 | 1.079062 | 1.078008 |
| 45 | 5 | 1 | | 1.077536 | 1.077825 | 1.078406 | 1.077355 |
| 46 | 4 | | | 1.078913 | 1.082783 | 1.083927 | 1.082783 |
| 47 | 4 | 1 | * | 1.082169 | 1.082901 | 1.084055 | 1.082901 |
| 48 | 3 | | | 1.079121 | 1.077900 | 1.078953 | 1.077900 |
| 49 | 4 | | | 1.078569 | 1.079637 | 1.080729 | 1.079637 |
| 50 | 4 | | | 1.079304 | 1.077224 | 1.078262 | 1.077224 |
| 51 | 4 | | | 1.079421 | 1.077484 | 1.078528 | 1.077484 |
| 52 | 3 | | | 1.080193 | 1.079057 | 1.080134 | 1.079057 |
| 53 | 4 | | * | 1.079334 | 1.077190 | 1.078231 | 1.077190 |
| 54 | 4 | 1 | * | 1.078151 | 1.077662 | 1.076424 | 1.075370 |
| 55 | 2 | | | 1.077803 | 1.080367 | 1.081472 | 1.080367 |
| 56 | 3 | | * | 1.078780 | 1.082377 | 1.083524 | 1.082377 |
| 57 | 2 | | | 1.077935 | 1.077329 | 1.078373 | 1.077329 |
| 58 | 6 | | * | 1.078393 | 1.076933 | 1.077970 | 1.076933 |
| 59 | 2 | | | 1.078965 | 1.077468 | 1.078514 | 1.077468 |
| 60 | 2 | | | 1.078772 | 1.079179 | 1.080260 | 1.079179 |
| 61 | 4 | | * | 1.083053 | 1.081217 | 1.082338 | 1.081217 |
| 62 | 6 | | * | 1.078518 | 1.081005 | 1.082122 | 1.081005 |
| 63 | 4 | 1 | * | 1.082441 | 1.078668 | 1.079733 | 1.078661 |
| 64 | 4 | | | 1.078863 | 1.077704 | 1.078753 | 1.077704 |
| 65 | 2 | | | 1.078813 | 1.078464 | 1.079529 | 1.078464 |
| 66 | 4 | | | 1.077995 | 1.078267 | 1.079327 | 1.078267 |

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|---|---|---|---|---|---|---|---|
| 67 | 3 | | | 1.082142 | 1.078923 | 1.079999 | 1.078923 |
| 68 | 6 | | | 1.078992 | 1.078932 | 1.080008 | 1.078932 |
| 69 | 5 | | | 1.078494 | 1.078809 | 1.079879 | 1.078809 |
| 70 | 7 | 1 | | 1.082392 | 1.078127 | 1.078241 | 1.077182 |
| 71 | 3 | | | 1.082071 | 1.077036 | 1.078073 | 1.077036 |
| 72 | 5 | | * | 1.077754 | 1.077141 | 1.078180 | 1.077141 |
| 73 | 5 | | | 1.082265 | 1.077823 | 1.078873 | 1.077823 |
| 74 | 3 | | | 1.077839 | 1.078174 | 1.079233 | 1.078174 |
| 75 | 4 | | | 1.080175 | 1.078806 | 1.079880 | 1.078806 |
| 76 | 4 | 1 | | 1.078930 | 1.078183 | 1.077440 | 1.076381 |
| 77 | 6 | | | 1.077284 | 1.077813 | 1.078865 | 1.077813 |
| 78 | 2 | | * | 1.078194 | 1.084571 | 1.085763 | 1.084571 |
| 79 | 5 | | | 1.082461 | 1.078625 | 1.079694 | 1.078625 |
| 80 | 5 | | * | 1.087466 | 1.082574 | 1.083723 | 1.082574 |
| 81 | 3 | 1 | * | 1.087516 | 1.080770 | 1.081882 | 1.080769 |
| 82 | 4 | | | 1.078959 | 1.081575 | 1.082697 | 1.081575 |
| 83 | 0 | | | 1.082559 | 1.075715 | 1.076724 | 1.075715 |
| 84 | 4 | | | 1.076912 | 1.079057 | 1.080135 | 1.079057 |
| 85 | 5 | | * | 1.077580 | 1.081825 | 1.082957 | 1.081825 |
| 86 | 7 | 2 | * | 1.081262 | 1.081597 | 1.080911 | 1.079783 |
| 87 | 6 | | | 1.083027 | 1.079756 | 1.080848 | 1.079756 |
| 88 | 2 | | | 1.078397 | 1.079149 | 1.080229 | 1.079149 |
| 89 | 5 | | * | 1.079351 | 1.076985 | 1.078021 | 1.076985 |
| 90 | 2 | | | 1.078624 | 1.078063 | 1.079121 | 1.078062 |
| 91 | 4 | | * | 1.078874 | 1.082102 | 1.083239 | 1.082102 |
| 92 | 3 | | * | 1.078489 | 1.081387 | 1.082512 | 1.081387 |
| 93 | 6 | | * | 1.082627 | 1.081307 | 1.082432 | 1.081307 |
| 94 | 1 | | | 1.080301 | 1.076993 | 1.078029 | 1.076993 |
| 95 | 2 | | | 1.080130 | 1.077863 | 1.078916 | 1.077863 |
| 96 | 4 | | * | 1.082969 | 1.085721 | 1.086936 | 1.085721 |
| 97 | 3 | | | 1.083676 | 1.076895 | 1.077927 | 1.076895 |
| 98 | 4 | | | 1.082684 | 1.080131 | 1.081230 | 1.080131 |
| 99 | 4 | | | 1.079258 | 1.076934 | 1.077964 | 1.076934 |
| 100 | 4 | | | 1.080809 | 1.078171 | 1.079230 | 1.078171 |
| 101 | 3 | | | 1.077630 | 1.077863 | 1.078916 | 1.077863 |
| 102 | 5 | | | 1.079084 | 1.077914 | 1.078968 | 1.077914 |
| 103 | 5 | | * | 1.080143 | 1.077556 | 1.078605 | 1.077556 |
| 104 | 4 | | | 1.077978 | 1.078115 | 1.079173 | 1.078115 |
| 105 | 5 | | * | 1.081513 | 1.081887 | 1.083022 | 1.081887 |
| 106 | 4 | | | 1.082640 | 1.077668 | 1.078717 | 1.077668 |

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|---|---|---|---|---|---|---|---|
| 107 | 5 | 3 | * | 1.081664 | 1.081603 | 1.082363 | 1.081234 |
| 108 | 4 | 2 | * | 1.082336 | 1.081561 | 1.082067 | 1.080940 |
| 109 | 3 | 1 | * | 1.081688 | 1.082014 | 1.078638 | 1.077507 |
| 110 | 4 | | | 1.078171 | 1.081189 | 1.082310 | 1.081189 |
| 111 | 3 | | | 1.082514 | 1.077899 | 1.078953 | 1.077899 |
| 112 | 4 | | * | 1.083292 | 1.081331 | 1.082455 | 1.081331 |
| 113 | 3 | | * | 1.082283 | 1.077634 | 1.078682 | 1.077634 |
| 114 | 3 | | * | 1.080503 | 1.081784 | 1.082916 | 1.081784 |
| 115 | 4 | | * | 1.078350 | 1.077453 | 1.078497 | 1.077453 |
| 116 | 4 | | * | 1.079776 | 1.081768 | 1.082900 | 1.081768 |
| 117 | 4 | | * | 1.078653 | 1.077409 | 1.078455 | 1.077409 |
| 118 | 4 | | * | 1.079084 | 1.076764 | 1.077795 | 1.076764 |
| 119 | 3 | 19 | * | 1.078724 | 1.085176 | 1.038021 | 1.037016 |
| 120 | 4 | | | 1.082778 | 1.077344 | 1.078386 | 1.077344 |
| 121 | 4 | | | 1.083262 | 1.077265 | 1.078306 | 1.077265 |
| 122 | 3 | 1 | * | 1.080102 | 1.081558 | 1.082488 | 1.081360 |
| 123 | 5 | 1 | * | 1.080131 | 1.077521 | 1.076945 | 1.075901 |
| 124 | 5 | 1 | | 1.078094 | 1.077499 | 1.069673 | 1.068629 |
| 125 | 4 | | | 1.082833 | 1.077794 | 1.078846 | 1.077794 |
| 126 | 4 | | | 1.080821 | 1.117970 | 1.078878 | 1.077824 |
| 127 | 5 | 1 | * | 1.081423 | 1.081750 | 1.077785 | 1.076657 |
| 128 | 4 | | * | 1.081174 | 1.081433 | 1.082558 | 1.081433 |
| 129 | 4 | | | 1.077372 | 1.077713 | 1.078761 | 1.077713 |
| 130 | 4 | 1 | | 1.083118 | 1.080808 | 1.078727 | 1.077619 |
| 131 | 5 | | | 1.080156 | 1.079096 | 1.080175 | 1.079096 |
| 132 | 5 | 1 | | 1.084994 | 1.078868 | 1.073107 | 1.072041 |
| 133 | 4 | 2 | * | 1.084326 | 1.081145 | 1.075363 | 1.074250 |
| 134 | 4 | | * | 1.081849 | 1.081156 | 1.082276 | 1.081156 |
| 135 | 3 | | * | 1.084632 | 1.081832 | 1.082965 | 1.081832 |
| 136 | 4 | 1 | | 1.080815 | 1.078806 | 1.078250 | 1.077181 |
| 137 | 2 | | | 1.080038 | 1.078284 | 1.079345 | 1.078284 |
| 138 | 4 | 2 | | 1.078593 | 1.078560 | 1.079404 | 1.078337 |
| 139 | 3 | | | 1.079721 | 1.078868 | 1.079944 | 1.078868 |
| 140 | 3 | | | 1.079498 | 1.079272 | 1.080354 | 1.079272 |
| 141 | 5 | | | 1.078062 | 1.079983 | 1.081081 | 1.079983 |
| 142 | 4 | | * | 1.079899 | 1.076807 | 1.077840 | 1.076807 |
| 143 | 5 | | | 1.079350 | 1.077708 | 1.078757 | 1.077708 |
| 144 | 4 | | | 1.079062 | 1.077192 | 1.078233 | 1.077192 |
| 145 | 5 | | * | 1.078876 | 1.076511 | 1.077536 | 1.076511 |
| 146 | 5 | | | 1.083927 | 1.077860 | 1.078913 | 1.077860 |

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|---|---|---|---|---|---|---|---|
| 147 | 5 | 1 | * | 1.084055 | 1.081051 | 1.081420 | 1.080303 |
| 148 | 5 | | | 1.078953 | 1.078064 | 1.079121 | 1.078064 |
| 149 | 4 | | | 1.080729 | 1.077524 | 1.078569 | 1.077524 |
| 150 | 4 | | | 1.078262 | 1.078244 | 1.079304 | 1.078244 |
| 151 | 4 | | | 1.078528 | 1.078358 | 1.079421 | 1.078358 |
| 152 | 5 | | | 1.080134 | 1.079113 | 1.080193 | 1.079113 |
| 153 | 3 | | | 1.078231 | 1.078273 | 1.079334 | 1.078273 |
| 154 | 4 | | | 1.078718 | 1.077116 | 1.078151 | 1.077116 |
| 155 | 5 | | | 1.081472 | 1.076771 | 1.077803 | 1.076771 |
| 156 | 6 | 1 | | 1.083524 | 1.077730 | 1.078770 | 1.077720 |
| 157 | 5 | | | 1.078373 | 1.076902 | 1.077935 | 1.076902 |
| 158 | 5 | | | 1.077970 | 1.077352 | 1.078393 | 1.077352 |
| 159 | 5 | | | 1.078514 | 1.077912 | 1.078965 | 1.077912 |
| 160 | 4 | | | 1.080260 | 1.077722 | 1.078772 | 1.077722 |
| 161 | 4 | | * | 1.082338 | 1.081917 | 1.083053 | 1.081917 |
| 162 | 6 | 1 | | 1.082122 | 1.077470 | 1.074838 | 1.073795 |
| 163 | 5 | | * | 1.079741 | 1.081317 | 1.082441 | 1.081316 |
| 164 | 6 | | | 1.078753 | 1.077812 | 1.078863 | 1.077812 |
| 165 | 5 | | | 1.079529 | 1.077760 | 1.078813 | 1.077760 |
| 166 | 6 | | * | 1.079327 | 1.076960 | 1.077995 | 1.076960 |
| 167 | 5 | 3 | * | 1.079999 | 1.081022 | 1.077919 | 1.076805 |
| 168 | 6 | 1 | * | 1.080008 | 1.077932 | 1.076262 | 1.075204 |
| 169 | 5 | | * | 1.079879 | 1.077444 | 1.078494 | 1.077444 |
| 170 | 6 | 1 | * | 1.079186 | 1.081268 | 1.081857 | 1.080734 |
| 171 | 6 | | * | 1.078073 | 1.080954 | 1.082071 | 1.080954 |
| 172 | 5 | | * | 1.078180 | 1.076722 | 1.077754 | 1.076722 |
| 173 | 5 | 2 | * | 1.078873 | 1.081144 | 1.074379 | 1.073267 |
| 174 | 4 | | * | 1.079233 | 1.076806 | 1.077839 | 1.076806 |
| 175 | 4 | | | 1.079880 | 1.079096 | 1.080175 | 1.079096 |
| 176 | 4 | 1 | | 1.079245 | 1.077876 | 1.074633 | 1.073583 |
| 177 | 5 | | * | 1.078865 | 1.076262 | 1.077284 | 1.076262 |
| 178 | 5 | | | 1.085763 | 1.077158 | 1.078194 | 1.077158 |
| 179 | 3 | | * | 1.079694 | 1.081337 | 1.082461 | 1.081337 |
| 180 | 4 | | * | 1.083723 | 1.086243 | 1.087466 | 1.086243 |
| 181 | 3 | | * | 1.081882 | 1.086291 | 1.087516 | 1.086291 |
| 182 | 3 | | * | 1.082697 | 1.077903 | 1.078959 | 1.077903 |
| 183 | 4 | | * | 1.076724 | 1.081432 | 1.082559 | 1.081432 |
| 184 | 3 | | * | 1.080135 | 1.075897 | 1.076912 | 1.075897 |
| 185 | 6 | | | 1.082957 | 1.076549 | 1.077580 | 1.076549 |
| 186 | 6 | | | 1.082727 | 1.080162 | 1.081262 | 1.080162 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 187 | 4 | | 1.080848 | 1.081901 | 1.083027 | 1.081901 |
| 188 | 5 | | 1.080229 | 1.077355 | 1.078397 | 1.077355 |
| 189 | 5 | | 1.078021 | 1.078289 | 1.079351 | 1.078289 |
| 190 | 4 | * | 1.079121 | 1.077569 | 1.078624 | 1.077569 |
| 191 | 4 | | 1.083239 | 1.077822 | 1.078874 | 1.077822 |
| 192 | 4 | | 1.082512 | 1.077443 | 1.078489 | 1.077443 |
| 193 | 5 | * | 1.082432 | 1.081500 | 1.082627 | 1.081500 |
| 194 | 3 | | 1.078029 | 1.079222 | 1.080301 | 1.079222 |
| 195 | 3 | | 1.078916 | 1.079052 | 1.080130 | 1.079052 |
| 196 | 3 | * | 1.086936 | 1.081835 | 1.082969 | 1.081835 |
| 197 | 4 | * | 1.077927 | 1.082527 | 1.083676 | 1.082527 |
| 198 | 5 | * | 1.081230 | 1.081556 | 1.082684 | 1.081556 |
| 199 | 5 | | 1.077964 | 1.078199 | 1.079258 | 1.078199 |
| 200 | 4 | | 1.079229 | 1.079717 | 1.080810 | 1.079718 |

* structure omitted from ensemble of 122 RS configurations for isotopic substitution in cyanide anion